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Dissipative Quantum Systems
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Flow Equations

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Dissipative Quantensysteme und Flussgleichungen

Die vorliegende Arbeit untersucht dissipative Quantensysteme mithilfe von Flussgleichungen für Hamiltonoperatoren. Ausgangspunkt stellt das Spin-Boson-Modell mit einer bosonischen Mode dar. Die Flussgleichungsresultate für die Grundzustandsenergie und für die Transformation der Pauli Spinmatrizen werden dabei mit der numerisch exakten Lösung verglichen. Für das Spin-Boson-Modell mit beliebiger Anzahl bosonischer Moden und explizit gebrochener Spiegelsymmetrie werden allgemeine Flussgleichungen aufgestellt, wobei ein Trunkierungsschema mit ℓ-abhängiger Normalordnung eingeführt wird. Wir beobachten universelles asymptotisches Verhalten und geben eine Diskussion. Abschliessend wird ein Brownsches Teilchen in einem periodischen Potential mit gebrochener Spiegelsymmetrie betrachtet, wobei die Methodik der vorherigen Abschnitte verwendet wird. In diesem Zusammenhang werden auch Resultate für das Tomonaga-Luttinger-Modell mit Störstelle gegeben.

Dissipative Quantum Systems and Flow Equations

This work investigates dissipative quantum systems by means of Flow Equations for Hamiltonians. We start with the Spin-Boson Model including one bosonic mode. The Flow Equation results for the ground-state energy and for the transformation of the Pauli spin matrices are compared with the numerically exact solution. For the Spin-Boson Model with an arbitrary number of bosonic modes and explicitly broken reflection symmetry, general Flow Equations are set up using a truncation scheme which involves an ℓ-dependent normal ordering procedure. Furthermore, observations on universal asymptotic behaviour are discussed. The remaining chapter investigates quantum Brownian motion in a periodic potential with broken reflection symmetry - employing the previous procedures. In this context we also include results for the Tomonaga-Luttinger Model with impurity.

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1. Introduction

Non-perturbative methods resemble an invaluable tool for the theoretical analysis of many-body systems and often yield the only reliable results available. Yet their number is limited, and especially exact methods are generally only applicable to a confined parameter regime or to specific models. The refermionization technique e.g. only works at the so-called Toulouse point while Bethe-ansatz techniques are limited to integrable models.

In 1993 and 1994 a new non-perturbative method was proposed by Wilson and Glazek and independently by Wegner. Whereas in high energy physics the method is known as *Similarity Transformations*, the term *Flow Equations* has been established in the solid-state community.

The idea is conceptionally simple: Instead of diagonalizing the Hamiltonian of the system by a single unitary transformation, one performs a continuous sequence of infinitesimal unitary transformations and thus induces a flow on the system parameters. The procedure is not constrained to specific symmetries nor to certain parameter regimes - but is accessible to any system described by a Hamiltonian. Thus, the method has been successfully applied to various models of solid-state and nuclear physics.

Since the method is strikingly simple it allows great freedom in its applications. Yet one is always in search of a distinguished scheme and in addition, to justify certain approximations and *ansätze*. Approximations become necessary as the Flow Equations usually create an infinite hierarchy of newly generated interaction terms. One therefore calls for a suitable and objective truncation scheme.

This work will address these questions when applied to *Dissipative Quantum Systems*. For dissipative systems the bath parameters are left invariant during the flow, which is intuitively apparent since the system should not have any effect on the infinite bath. Therefore, they serve as an ideal testing ground for the method. Still, they bear physical relevance and - amongst others - the question of quantum mechanical noise induced transport is currently debated in the literature. Furthermore, there is some controversy on the system behaviour when exposed to a sub-Ohmic bath.

One objective of this work is to propose a general truncation scheme, which leads to Flow Equations that are invariant with respect to the initial Hamiltonian up to a unitary transformation. Further, emphasis is placed on the aspect of symmetry breaking in the initial Hamiltonian and during the operator flow. We end up with an objective ℓ-dependent truncation scheme which can also be applied to other systems, such as electron-phonon systems where both system parameters will flow.

This work is organized such that all sections are more or less self-contained. References to previous sections are avoided and no specific knowledge is required for each section so that one can basically skip to the topic of interest. The price is a sometimes redundant introduction to the several models.

This work is also hierarchical in the sense that we start with a rudimentary Hamiltonian and add further contributions as we go along. This is done from two perspectives, firstly considering a bosonic bath; and secondly considering a fermionic bath. This work is divided into the following chapters:

The second chapter deals with exactly solvable models: The *Independent Boson Model* to justify the expansion of fermionic operators into an infinite series of unbounded operators; and the *Dissipative Harmonic Oscillator* to introduce the general scheme how to treat dissipative quantum systems within the Flow Equation approach. We also consider the *Tomonaga-Luttinger Model* to point out that the specific representation of operators becomes crucial in the Flow Equation approach and to lay ground for later extensions of the model.

The third chapter then deals with the Spin-Boson Model with only one bosonic mode. Throughout this work we refer to this model as the *Rabi Model* in order to avoid confusion with the *Spin-Boson Model* with an arbitrary number of modes and arbitrary dispersion, discussed in Chapter 4. Different truncation schemes are tested and compared with the numerically exact solution that is obtained for the ground-state energy and for the fixed point operator of the observable flow. In order to compare the fixed point operator with the Flow Equation result, a unique composition of the fixed point matrix is presented.

The forth chapter deals with the simplest non-trivial dissipative quantum system, the *Spin-Boson Model*. Emphasis is placed on breaking the reflection symmetry and a general truncation scheme is proposed. Furthermore, we investigate Flow Equations where all system parameters tend to zero for the fixed point Hamiltonian and display universal asymptotic behaviour.

The fifth chapter deals with *Brownian Motion in a Periodic Potential* where the focus is again on a reflection-breaking periodic potential. The previously developed procedures prove to be easily applicable to this extended dissipative model. Finally the Tomonaga-Luttinger Model with impurity is considered.

We close with a *Summary and Outlook*.

Throughout this work we set $\hbar = 1$.

2. Exactly Solvable Models

Prior to the application of Flow Equations to exactly solvable models, a brief introduction to the method itself is as follows:

- Consider a family of unitarily equivalent Hamiltonians ($U^\dagger(\ell) = U^{-1}(\ell)$, $\ell \in \mathbb{R}_0^+$)

$$H(\ell) = U(\ell) H U^\dagger(\ell) \quad .$$

- Differentiating both sides, the infinitesimal version reads

$$\partial_\ell H = [\eta, H] \quad , \quad \text{with } \eta = -U(\ell)\partial_\ell U^\dagger(\ell) \quad .$$

- The choice $\eta = [H_0, V]$ will diagonalize the Hamiltonian $H = H_0 + V$ for $\ell \to \infty$. By diagonalizing is meant that the trace of the square of the off-diagonal matrix elements V is monotonically decreasing for increasing ℓ, i.e. $\partial_\ell(\mathrm{tr}V^2) \leq 0$ [Weg94].

In the following chapters the choice $\eta = [H_0, V]$ will be called the *canonical* generator. But it is by no means the unique nor invariably the best choice. For example, instead of focusing on the trace of the square of the off-diagonal matrix elements, Wegner introduced a general functional of the Hamiltonian under consideration, that is subjected to reach its minimum during the flow [Gro01]. For banded matrices, Mielke proposed that the flow should preserve the structure of the initial Hamiltonian that demands a generator which also differs from the canonical choice [Mie98]. Another strategy is to start with the canonical generator and then add further contributions to the generator with the objective to cancel interaction terms that were created by the canonical choice [Keh97].

The Flow Equation approach allows great freedom. To obtain a qualitative and quantitative picture, we consider a real, symmetric 2×2 matrix with trace zero. The matrix is thus characterized by two parameters; the diagonal part d_0 and the off-diagonal part e_0. Postulating that the Flow Equations shall diagonalize the matrix for $\ell \to \infty$ all functions $e(\ell)$ with $e(0) = e_0$ and $e(\ell) \to 0$ for $\ell \to \infty$ are allowed, all corresponding to a different generator η and to a different function $d(\ell)$. Nevertheless the functions $d(\ell)$ have the same limiting value $d(\ell) \to d^*$ for $\ell \to \infty$ if no approximation is made.

Even though all different Flow Equations are equivalent and will eventually lead to the same result, matters change as soon as approximations are involved. Then a systematic decoupling is favorable. This is the second virtue of the canonical choice $\eta = [H_0, V]$ apart from diagonalizing the system: States with high energy difference are decoupled first. More precisely, the scale of energy difference just being decoupled is given by $\ell^{-1/2}$.[1] The separation of energy scales is a basic feature of the renormalization group. The Flow Equation approach is therefore likely to describe systems that were previously only tractable by "conventional" renormalization group techniques based on functional integrals and effective actions.

We would like to make a second comment which involves the choice of the diagonal part H_0. Principally, there is no constraint for choosing an appropriate diagonal Hamiltonian; even though it is often best to choose the "largest" one still diagonalizable [Ric97]. The only condition is that the spectrum of H_0 and H are principally of the same kind. For example, choosing the kinetic part of the Hamiltonian of the harmonic oscillator as diagonal Hamiltonian will not lead to the correct spectrum; instead considering a harmonic potential as perturbation to the harmonic oscillator will give the desired solution.

With these preliminary remarks we are now set to apply Flow Equations to exactly solvable models. We will especially focus on the similarities of the models discussed in the following chapters. Therefore some of the notations and various points discussed will become clearer when reading the next chapters.

2.1. Independent Boson Model

The Independent Boson Model is given by the Hamiltonian

$$H = H_0 + V = \omega b^\dagger b + \epsilon c^\dagger c + \lambda c^\dagger c(b + b^\dagger) \quad . \tag{2.1}$$

The $b^{(\dagger)}$ resemble bosonic, the $c^{(\dagger)}$ fermionic operators. They obey the canonical commutation and anti-commutation relations respectively. The model can account for some relaxation phenomena and is extensively discussed in the textbook by Mahan [Mah90].

We set $\epsilon = \lambda^2/\omega$. Then the Hamiltonian of Eq. (2.1) is equivalent to $H = \omega b^\dagger b + \sigma_z \lambda(b + b^\dagger)$, where σ_z denotes the z-component of the Pauli spin matrices. We will encounter this latter form of the Hamiltonian in Chapter 3, where we will add an additional term that will couple the two fermionic states through the tunnel-matrix $-\frac{\Delta}{2}\sigma_x$.

The model is easily solved by the unitary transformation

$$U = \exp(-c^\dagger c \frac{\lambda}{\omega}(b - b^\dagger)) \tag{2.2}$$

[1] Glazek and Wilson do not focus on the absolute but relative energy difference in their Similarity Transformations [Gla94]. Mielke showed a certain equivalence of the two schemes [Mie97].

and we obtain the diagonalized Hamiltonian $UHU^\dagger = \omega b^\dagger b$.

But we want to perform this unitary transformation continuously by introducing a flow parameter ℓ and a family of unitarily equivalent Hamiltonians $H(\ell) = U(\ell)HU^\dagger(\ell)$. We also want to look closely at the transformed operator $c(\ell) \equiv U(\ell)cU^\dagger(\ell)$ and question if an expansion of the operator in a series of unbounded operators, namely $(b - b^\dagger)^n$, is well-defined. Further, we want to study which effects a truncation of the series might have on the unitarity of the transformation, i.e. we want to observe how quantities which are conserved under unitary transformations - like commutator relations - are changing.

The unitary operators $U(\ell)$ shall be defined by the generator η which governs the differential form of a continuous unitary transformations as follows: $\partial_\ell H = [\eta, H]$. A good choice for the generator has proven to be $\eta = [H_0, V]$, which is likely to eliminate the interaction in the limit $\ell \to \infty$. The ℓ-dependent unitary operator $U(\ell)$ is related to the generator η through the differential equation $\partial_\ell U = \eta U$ which can be formally integrated to yield $U(\ell) = L\exp(\int_0^\ell d\ell' \eta(\ell'))$. The operator L denotes the ℓ-ordering operator, defined in the same way as the more familiar time-ordering operator T. In fact, the differential form of the Flow Equations has got the same structure as the Heisenberg equation of motion.

For the independent boson model the canonical generator reads $\eta = -\omega\lambda c^\dagger c(b - b^\dagger)$ and we readily obtain

$$[\eta, H] = -\omega^2\lambda c^\dagger c(b + b^\dagger) - 2\omega\lambda^2 c^\dagger c \quad . \tag{2.3}$$

The following Flow Equations

$$\partial_\ell \lambda = -\omega^2\lambda \quad , \quad \partial_\ell \epsilon = -2\omega\lambda^2 \tag{2.4}$$

are integrated to yield $\lambda(\ell) = \lambda\exp(-\omega^2\ell)$ and $\epsilon(\ell) = \frac{\lambda^2}{\omega}\exp(-2\omega^2\ell)$. Since $[\eta(\ell), \eta(\ell')] = 0$, the ℓ-ordering operator L becomes trivial and we obtain for the ℓ-dependent unitary operator

$$U(\ell) = \exp(-c^\dagger c\frac{\lambda}{\omega}(1 - e^{-\omega^2\ell})(b - b^\dagger)) \quad . \tag{2.5}$$

From Eq. (2.5) we can obtain the unique unitary operator for $\ell \to \infty$ which diagonalizes H and which was already given in Eq. (2.2).

Given $U(\ell)$ one can determine the flow of the operator $c(\ell)$ directly:

$$c(\ell) = U(\ell)cU^\dagger(\ell) = c\exp(\frac{\delta\lambda(\ell)}{\omega}(b - b^\dagger)) \tag{2.6}$$

$$= c\exp(-\frac{1}{2}\left(\frac{\delta\lambda(\ell)}{\omega}\right)^2)\exp(-\frac{\delta\lambda(\ell)}{\omega}b^\dagger)\exp(\frac{\delta\lambda(\ell)}{\omega}b) \tag{2.7}$$

$$\equiv c\exp(-\frac{1}{2}\left(\frac{\delta\lambda(\ell)}{\omega}\right)^2)\sum_{n=0}\left(\frac{\delta\lambda(\ell)}{\omega}\right)^n\frac{:(b - b^\dagger)^n:}{n!} \quad , \tag{2.8}$$

where we introduced $\delta\lambda(\ell) = \lambda(1 - e^{-\omega^2 \ell})$ and defined normal ordering, denoted by $: ... :$, by writing the creation operator left from the annihilation operator.[2]

We now apply the continuous transformation to the operator c using the differential form $\partial_\ell c = [\eta, c]$. The Flow Equations generate the infinite series $c(\ell) = c\sum_{n=0}\gamma_n(\ell)(b - b^\dagger)^n$ with $\partial_\ell \gamma_{n+1} = \omega\lambda(\ell)\gamma_n$. Together with the initial condition $\gamma_0 = 1$, $\gamma_n = 0$ for $n \geq 1$, this set of differential equations can be solved to yield $\gamma_n = \frac{1}{n!}(\frac{\delta\lambda(\ell)}{\omega})^n$. The Flow Equation result thus coincides with the non-normal ordered form of $c(\ell)$ in Eq. (2.6) if one expands the exponential function into a Taylor-series.

At first sight there is no distinguished expansion of $c(\ell)$ in bosonic operators since its generation depends on η. In order to discuss a different scheme, we now define $c(\ell)$ by a series of normal ordered operators, i.e. $c(\ell) = c\sum_{n=0}\gamma_n(\ell){:}\,(b - b^\dagger)^n\,{:}$. We obtain the following Flow Equations

$$\partial_\ell \gamma_{n+1} = \omega\lambda(\ell)(\gamma_n - (n+2)\gamma_{n+2}) \quad , \tag{2.9}$$

where we used the formula (see Appendix A)

$$(b - b^\dagger) : (b - b^\dagger)^n :=: (b - b^\dagger)^{n+1} : +n\langle (b - b^\dagger)^2\rangle : (b - b^\dagger)^{n-1} : \tag{2.10}$$

at $T = 0$, i.e. $\langle (b - b^\dagger)^2\rangle = -1$ with $\langle ... \rangle$ denoting the bosonic ground-state expectation value. Taking the same initial conditions as in the case of the non-normal ordered expansion, we see that the normal ordered expansion in Eq. (2.8) solves the set of differential equations (2.9), i.e. $\gamma_n = \exp(-\frac{1}{2}(\delta\lambda(\ell)/\omega)^2)\frac{1}{n!}(\frac{\delta\lambda(\ell)}{\omega})^n$.

This is a remarkable result. Whereas the non-normal ordered expansion of $c(\ell)$ reproduces the perturbative result in the coupling $\delta\lambda$ for each coefficient γ_n, the normal ordered expansion yields coefficients γ_n, which contain all powers of $\delta\lambda$. Especially in view of later approximations, the normal ordered version will then be more preferable, since it is likely to go beyond a perturbative description.

After having recovered the correct flow of the observable via the Flow Equation approach, we would like to investigate the "stability" of the infinite expansion of $c(\ell)$ in unbounded operators. For this purpose, we consider the Green function $G(t) = -i\langle Tc(t)c^\dagger\rangle$ and the spectral function $A(\tilde{\omega}) = -\mathrm{Im}G(\tilde{\omega})/\pi$ with the time ordering operator T, the Fourier transform $G(\tilde{\omega}) = \int dt e^{i\tilde{\omega}t}G(t)$ and $\langle \ldots \rangle$ denoting the ground-state expectation value with respect to H. With $\tilde{\lambda} \equiv \lambda/\omega$ we obtain [Mah90]

$$G(t) = -i\Theta(t)\exp(-\tilde{\lambda}^2(1 - e^{-i\omega t})) \quad , \tag{2.11}$$

$$A(\tilde{\omega}) = e^{-\tilde{\lambda}^2}\sum_{n=0}\tilde{\lambda}^{2n}\frac{1}{n!}\delta(\tilde{\omega} - n\omega) \quad . \tag{2.12}$$

[2]This definition of normal ordering resembles a special case of the general definition given in Appendix A and is valid at $T = 0$. But from now on the general definition will be used.

The spectral function $A(\tilde{\omega})$ thus exhibits the polaronic shift $\epsilon_p = -\lambda^2/\omega$ for $n = 0$ and an equidistant satellite structure separated by the oscillator frequency ω with exponentially decreasing weight.

Using Flow Equations, the Green function is best expressed as

$$G(t) = -i\Theta(t)\langle e^{iH(\ell=\infty)t}c^\dagger(\ell=\infty)e^{-iH(\ell=\infty)t}c(\ell=\infty)\rangle \quad , \tag{2.13}$$

because then the time evolution of the fermionic and bosonic operator becomes trivial.

In order to recover the exact result, we first use the normal ordered expansion of $c(\ell)$. With $D(t) \equiv b(t) - b^\dagger(t)$, where the time evolution is given by the Heisenberg representation with $H(\ell = \infty) = \omega b^\dagger b$, the Green function reads:

$$G(t) = -i\Theta(t)e^{-\tilde{\lambda}^2}\langle c(t)\sum_{n=0}\frac{\tilde{\lambda}^n}{n!} : D^n(t) : c^\dagger \sum_{m=0}\frac{\tilde{\lambda}^m}{m!}(-1)^m : D^m(0) :\rangle \tag{2.14}$$

$$= -i\Theta(t)e^{-\tilde{\lambda}^2}\sum_{n,m=0}\frac{\tilde{\lambda}^n}{n!}\frac{\tilde{\lambda}^m}{m!}(-1)^m\langle : D^n(t) :: D^m(0) :\rangle \tag{2.15}$$

$$= -i\Theta(t)e^{-\tilde{\lambda}^2}\sum_{n,m=0}\frac{\tilde{\lambda}^n}{n!}\frac{\tilde{\lambda}^m}{m!}n!\delta_{n,m}e^{-in\omega t} \tag{2.16}$$

To get from Eq. (2.15) to Eq. (2.16) we used the following formula (Appendix A):

$$: (b-b^\dagger)^n :: (b-b^\dagger)^m :=: \exp(\langle(b-b^\dagger)^2\rangle\frac{\partial^2}{\partial x_1\partial x_2})x_1^n x_2^m|_{x_1=x_2=(b-b^\dagger)} : \quad , \tag{2.17}$$

with $\langle(b-b^\dagger)^2\rangle = -1$ and $\langle : (b-b^\dagger)^n :\rangle = 0$ at $T = 0$. Summing up the series in Eq. (2.16) indeed yields the exact result given in Eq. (2.11).

In order to show that also the non-normal ordered expansion of $c(\ell)$ leads to the correct result, we have to normal order this expansion. For this we need the following formula (Appendix A):

$$(b-b^\dagger)^n = \sum_{k=0}^{[\frac{n-1}{2}]}\frac{1}{k!}\frac{n!}{2^k(n-2k)!}\langle(b-b^\dagger)^2\rangle^k : (b-b^\dagger)^{n-2k} : \tag{2.18}$$

Considering for the moment only the first $(N+1)$ even powers of $(b-b^\dagger)$, we obtain

$$\sum_{n=0}^{N}\frac{\tilde{\lambda}^{2n}}{2n!}(b-b^\dagger)^{2n} = \sum_{n=0}^{N}\sum_{k=0}^{n}\frac{\tilde{\lambda}^{2k}}{2^k}\frac{G^k}{k!}\frac{\tilde{\lambda}^{2(n-k)}}{2(n-k)!} : (b-b^\dagger)^{2(n-k)} : \tag{2.19}$$

$$= \sum_{m=0}^{N}\frac{\tilde{\lambda}^{2m}}{2m!} : (b-b^\dagger)^{2m} : \sum_{k=0}^{N-m}\frac{\tilde{\lambda}^{2k}}{2^k}\frac{G^k}{k!} \quad , \tag{2.20}$$

where we introduced $G \equiv \langle (b-b^\dagger)^2\rangle$ and $m = n-k$, $\langle ... \rangle$ denoting the canonical ensemble average over a free bosonic system . The summation of the first $(N+1)$ odd powers of $(b-b^\dagger)$ yields

$$\sum_{n=0}^{N} \frac{\tilde\lambda^{2n+1}}{(2n+1)!}(b-b^\dagger)^{2n+1} = \sum_{m=0}^{N} \frac{\tilde\lambda^{2m+1}}{(2m+1)!} : (b-b^\dagger)^{2m+1} : \sum_{k=0}^{N-m} \frac{\tilde\lambda^{2k}}{2^k}\frac{G^k}{k!} \quad . \tag{2.21}$$

In the limit $N\to\infty$ we obtain

$$\sum_{n=0} \frac{\tilde\lambda^n}{n!}(b-b^\dagger)^n = e^{\frac{1}{2}G\tilde\lambda^2} \sum_{n=0} \frac{\tilde\lambda^n}{n!} : (b-b^\dagger)^n : \quad , \tag{2.22}$$

which is an extension of the previous normal ordering of Eq. (2.8) to finite temperatures, since $G = -(1+n)$, $n \equiv (e^{\beta\omega}-1)^{-1}$ being the Bose factor. This shows that both expansions of $c(\ell)$ are equivalent.

To complete the discussion we will now verify that the anti-commutation relation $\{c(\ell), c^\dagger(\ell)\} = 1$ holds for all ℓ. To show this we will employ the non-normal ordered expansion. This yields:

$$\{c(\ell), c^\dagger(\ell)\} = \frac{1}{2}\sum_{n,n'=0} \gamma_n\gamma_{n'}((-1)^n + (-1)^{n'})(b-b^\dagger)^{n+n'} \tag{2.23}$$

$$= \sum_{n=0}\sum_{k=0}^{2n} (-1)^k \gamma_{2n-k}\gamma_k (b-b^\dagger)^{2n} = 1 \tag{2.24}$$

In the end of this section we want to briefly address the question how approximations effect the flow of the operator and if they yield reasonable results. We will first consider the Flow Equations for the non-normal ordered expansion of $c(\ell)$. Truncating the series after the second term yields the following set of differential equations:

$$\frac{d\gamma_0}{d\ell} = 0 \quad , \quad \frac{d\gamma_1}{d\ell} = \omega\lambda(\ell)\gamma_0 \quad . \tag{2.25}$$

This leads us to $c(\ell) = c(1+\tilde\lambda(1-e^{-\omega^2\ell})(b-b^\dagger))$ and thus $G(t) = -i(1+\tilde\lambda^2 e^{-i\omega t})$. To discuss this result it is useful to present the spectral function $A(\tilde\omega) = \delta(\tilde\omega) + \tilde\lambda^2\delta(\tilde\omega-\omega)$.

The spectral function does not satisfy the sum rule $\int d\tilde\omega A(\tilde\omega) = 1$. This can be understood by noting that the canonical anti-commutation relations are not satisfied either even after having taken the expectation value: $\langle\{c^\dagger(\ell), c(\ell)\}\rangle = 1 - (\delta\lambda(\ell)/\omega)^2\langle(b-b^\dagger)^2\rangle = 1 + (\delta\lambda(\ell)/\omega)^2$. Neglecting terms which are quadratic in the coupling λ yields the correct perturbative result for $\lambda/\omega \ll 1$.

Now let us check the approximation where we close the series after the second term by neglecting the *normal ordered* bosonic bilinear operator. The Flow Equations then read

$$\frac{d\gamma_0}{d\ell} = -\omega\lambda(\ell)\gamma_1 \quad , \quad \frac{d\gamma_1}{d\ell} = \omega\lambda(\ell)\gamma_0 \quad . \tag{2.26}$$

Defining $\vec{\gamma} \equiv (\gamma_0, \gamma_1)^T$ we obtain $\vec{\gamma}(\ell) = \exp(-i\lambda(\ell)\sigma_y \ell)\vec{\gamma}_0$ with σ_y denoting the y-component of the Pauli spin matrices and $\vec{\gamma}_0 = (1,0)^T$, which yields $c(\ell) = c(\cos(\lambda(\ell)\ell/\omega) - \sin(\lambda(\ell)\ell/\omega)(b - b^\dagger))$. This time the anti-commutation relation $\{c(\ell), c^\dagger(\ell)\} = \cos^2(\lambda(\ell)\ell/\omega) - \sin^2(\lambda(\ell)\ell/\omega)(b - b^\dagger)^2$ holds exactly after projecting it onto the ground-state. We obtain $A(\tilde{\omega}) = \delta(\tilde{\omega})$ and the sum rule thus holds.

We conclude that neglecting *normal ordered* operators yields more consistent results even though no qualitative improvement with respect to the non-normal ordered expansion was achieved. For this one has to include more terms.

We close this section with a summary of our results and conclusions. The series expansion of an operator into bosonic operators yields consistent results. This is no trivial result since expanding the bounded operator c into unbounded operators $(b - b^\dagger)^n$ might lead to inconsistencies. Further it has to be born in mind that the initial operator of the operator flow is resembled by $c(\ell = 0) = c \otimes 1_B$, with 1_B being the unity operator of the bosonic Hilbert space. One consequence then is that the trace of the initial operator is unbounded and thus not defined.

As a second result, we want to mention that both expansions, normal ordered and non-normal ordered, are equivalent if no approximations are involved. Nevertheless the operator expansion into *normal ordered* operators seems to be a distinguished expansion since it resembles a non-perturbative approach including the Debye-Waller factor and yields consistent results when approximations are involved.

2.2. Tomonaga-Luttinger Model

An instructive exactly solvable model is given by the Tomonaga-Luttinger (TL) Model. This model describes the low-energy properties of interacting fermions in one dimension in the high-density limit. In fact, it is closely related to the n-orbital model in one dimension on which Wegner introduced the method of Flow Equations [Weg94].

In the following section we will briefly derive the TL model starting from a one-dimensional interacting electron gas. We then give the solution of the TL model via Flow Equations including the transformation of the fermionic field, but where we make explicit use of the bosonization formula [Hal81]. In the last subsection we will transform the fermionic field based on the usual representation of fermionic ladder operators. The Flow Equations then generated an infinite hierarchy of operators so that approximations become necessary. The connection to dissipative quantum systems is established when one adds an impurity to the system and will be discussed in Chapter 5.

2.2.1. The Model

We start with the description of one-dimensional, non-relativistic, interacting spinless electrons on a ring of length L. The continuum version of the Hamiltonian reads

$$\begin{aligned} H = & \int_{-L/2}^{L/2} dx \psi^\dagger(x) \left(-\frac{\partial_x^2}{2m} \right) \psi(x) \\ & + \frac{1}{2} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} dx\, dx' \psi^\dagger(x) \psi^\dagger(x') U(x-x') \psi(x') \psi(x) \quad , \end{aligned} \tag{2.27}$$

where the fermionic field $\psi(x)$ obeys periodic boundary condition $\psi(-L/2) = \psi(L/2)$ and canonical anti-commutation relations $\{\psi(x), \psi^\dagger(x')\} = \delta(x-x')$. $U(x)$ resembles the two-body potential between the fermions. Performing the Fourier transformation with $\psi(x) = L^{-1/2} \sum_k e^{ikx} c_k$ and $U(x) = L^{-1} \sum_q e^{iqx} v_q$ the Hamiltonian is given by the following representation:

$$H = \sum_k \frac{k^2}{2m} c_k^\dagger c_k + \frac{1}{2L} \sum_{k,k',q} v_q c_{k-q}^\dagger c_{k'+q}^\dagger c_{k'} c_k \quad , \tag{2.28}$$

where $k, q = 2\pi n/L$, $n \in \mathbb{Z}$ and $c_k^{(\dagger)}$ creates (annihilates) the plane wave with wavenumber k.

Considering the high-density limit and focusing on the low-energy properties of the system, the energy dispersion can be linearized around the Fermi points $\pm k_F$ where $k_F = \pm 2\pi N/L$, N being the number of electrons. With the Fermi velocity $v_F \equiv k_F/m$

we obtain

$$H = v_F \sum_k |k| c_k^\dagger c_k + \frac{1}{2L} \sum_q v_q (\sum_k c_{k-q}^\dagger c_k)(\sum_{k'} c_{k'+q}^\dagger c_{k'}) \quad , \tag{2.29}$$

where we neglected terms that only contain the number-of-particle operator $\mathcal{N} \equiv \sum_k c_k^\dagger c_k$.

The system can now be decoupled into left- and right-moving fluctuations if we assume the interaction to be long-ranged in position space, i.e. $v_q/v_F \ll 1$ for $q \gg q_c$, where $q_c \ll k_F$ denotes the interaction cutoff [Tom50]. A less intuitive approach is to assume a delta-interaction in position space. A renormalization group analysis then shows that scattering processes from one branch to the other scale to zero, i.e. are irrelevant [Sol79]. The resulting Tomonaga-Luttinger Model thus resembles the fixpoint Hamiltonian of one-dimensional interacting electron systems.

A mathematically more rigorous treatment of the model with finite band cutoff is possible if the two branches of the linear dispersion are extended ranging from ∞ to $-\infty$. To assure a well-defined ground-state, the states with negative energy have then to be filled up with Dirac fermions. The creation and annihilation operators of the left- and right-moving fluctuations then obey exact bosonic commutation relations. These operators are defined as follows:

$$b_q^R \equiv n_q^{-1/2} \sum_k {c_{k-q}^R}^\dagger c_k^R \quad , \quad b_q^L \equiv n_q^{-1/2} \sum_k {c_{k+q}^L}^\dagger c_k^L \quad , \tag{2.30}$$

where $q > 0$ and $n_q \equiv Lq/(2\pi) \in \mathbb{N}$. We further introduced

$$c_k^R \equiv \begin{cases} c_k & k \geq 0 \\ d_k & k < 0 \end{cases} \quad , \quad c_k^L \equiv \begin{cases} c_k & k < 0 \\ d_k & k \geq 0 \end{cases} \quad . \tag{2.31}$$

The operators $d_k^{(\dagger)}$ create and annihilate the newly introduced Dirac fermions respectively. The commutation relation then reads $[b_q^i, {b_{q'}^{i'}}^\dagger] = \delta_{i,i'}\delta_{q,q'}$, with $i, i' = L, R$. In order to derive the commutation relation from the definition given in Eq. (2.30) one needs to normal order the fermionic operators with respect to the ground state of the Fermi-Dirac sea before changing the summation index.

The interaction term of the Hamiltonian given in Eq. (2.29) can now easily be expressed by the newly introduced bosonic operators. To do so also for the kinetic term, the Kronig-relation [Kro35] has to be employed:

$$\sum_k |k| c_k^\dagger c_k - \sum_k |k| d_k^\dagger d_k = \sum_{q>0} q({b_q^R}^\dagger b_q^R + {b_q^L}^\dagger b_q^L) + f(\mathcal{N}^L) + f(\mathcal{N}^R) \quad , \tag{2.32}$$

where $f(\mathcal{N}^{L/R})$ with $\mathcal{N}^{L/R} \equiv \sum_k {c_k^{L/R}}^\dagger c_k^{L/R}$ denotes a function of the number-of-particle operator of the left- and right-movers respectively. Again we will neglect these contributions. For a more detailed overview, see [Sch97] or [Del98].

We can now express the Hamiltonian completely through bosonic density-fluctuations:

$$\begin{aligned} H &= v_F \sum_{q>0} q\left(1+\frac{v_q}{2\pi v_F}\right)\left(b_q^{R\dagger} b_q^R + b_q^{L\dagger} b_q^L\right) \\ &+ \frac{1}{4\pi}\sum_{q>0} q v_q \left(b_q^R b_q^L + b_q^L b_q^R + b_q^{R\dagger} b_q^{L\dagger} + b_q^{L\dagger} b_q^{R\dagger}\right) \end{aligned} \tag{2.33}$$

One sees that the kinetic term is renormalized by scattering processes which conserve the energy, denoted as g_4-process in the g-ology model [Sol79]. These terms are to be identified with those terms that conserve the number of quasi-particles, as introduced by Wegner in Ref. [Weg94].[3] This shows that the Flow Equation approach is then successful if one chooses the "right" diagonal Hamiltonian corresponding to the distinguished basis.

2.2.2. Solution via Flow Equation

Since the Hamiltonian in Eq. (2.33) is bilinear in bosonic operators and only two different wave numbers q and $-q$ couple, diagonalization is straightforward via Bogoljubov transformation. But we want to diagonalize the Hamiltonian via Flow Equations. In order to abbreviate the notation we define $b_q \equiv b_q^R$ and $b_{-q} \equiv b_q^L$ for $q > 0$. The ℓ-dependent Hamiltonian then takes the following form:

$$H = \sum_{q\neq 0} \omega_q(\ell) b_q^\dagger b_q + \sum_{q\neq 0} v_q(\ell)\left(b_q b_{-q} + b_{-q}^\dagger b_q^\dagger\right) \equiv H_0 + V \tag{2.34}$$

The initial conditions are given by $\omega_q^0 \equiv \omega_q(\ell=0) = v_F|q|(1+v_q/2\pi v_F)$ and $v_q^0 \equiv v_q(\ell=0) = |q|v_q/4\pi$. The generator of the infinitesimal transformations is canonically defined as

$$\eta = [H_0, H] = -\sum_{q\neq 0} \omega_{-q}(v_q + v_{-q})\left(b_q b_{-q} - b_{-q}^\dagger b_q^\dagger\right) \quad , \tag{2.35}$$

which is likely to eliminate the interaction term V for $\ell \to \infty$.

The commutator $[\eta, H]$ yields the following contributions:

$$[\eta, H_0] = -\sum_{q\neq 0} \omega_{-q}(\omega_q + \omega_{-q})(v_q + v_{-q})\left(b_q b_{-q} + b_{-q}^\dagger b_q^\dagger\right) \tag{2.36}$$

$$[\eta, V] = -\sum_{q\neq 0} (\omega_q + \omega_{-q})(v_q + v_{-q})^2\left(b_q b_q^\dagger + b_q^\dagger b_q\right) \tag{2.37}$$

[3] Wegner included scattering terms to the diagonal Hamiltonian which conserve the number of electrons above and below the Fermi points.

Since $\omega_q(\ell = 0) = \omega_{-q}(\ell = 0)$, we have $\omega_q(\ell) = \omega_{-q}(\ell)$ and $v_q(\ell) = v_{-q}(\ell)$ for all ℓ. This shows that the Flow Equations preserve the symmetry between left- and right-movers. The Flow Equations $\partial_\ell H = [\eta, H]$ then read

$$\partial_\ell \omega_q = -16\omega_q v_q^2 \quad , \quad \partial_\ell v_q = -4\omega_q^2 v_q \quad . \tag{2.38}$$

Obviously $\omega_q^2 - 4v_q^2 = \text{const}$ and with $v_q(\ell = \infty) = 0$ we have $\tilde{\omega}_q \equiv \omega_q(\ell = \infty) = (\omega_q^2(\ell) - 4v_q^2(\ell))^{1/2}$. Inserting the initial conditions for $\ell = 0$ this yields the well-known result $\tilde{\omega}_q = v_F|q|\sqrt{1 + v_q/\pi v_F}$.

In order to investigate the flow of observables we need to know the ℓ-dependence of $\eta_q \equiv -2\omega_q v_q$. Since different wave numbers do not couple we will neglect the q-dependence of η_q for a moment and define $x = \omega_q v_q$ and $y = \omega_q^2 + 4v_q^2$. The set of differential equations for these variables reads:

$$\partial_\ell x = -4xy \quad , \quad \partial_\ell y = -64x^2 \tag{2.39}$$

From $\partial_\ell^2 y = -4\partial_\ell y^2$ we obtain the solution $y(\ell) = y_\infty \coth(4y_\infty \ell + C)$ with $\coth(C) = y(\ell = 0)/y_\infty$ and $y_\infty \equiv y(\ell = \infty)$. From the set of Eq. (2.39) one then obtains either $x(\ell) = y_\infty/(4\sinh(4y_\infty \ell + C))$ or $x(\ell) = x(\ell = 0)\sinh(C)/\sinh(4y_\infty \ell + C)$ which can only hold simultaneously if $y_\infty = 4x(\ell = 0)\sinh(C)$. Inserting the initial definitions one sees that this is indeed the case. We thus obtain

$$\eta_q(\ell) = -\frac{\tilde{\omega}_q^2}{2\sinh(4\tilde{\omega}_q^2 \ell + C_q)} \quad , \quad \text{with} \quad \sinh(C_q) = \frac{\tilde{\omega}_q^2}{4\omega_q^0 v_q^0} \quad . \tag{2.40}$$

We will further need the following indefinite integral:

$$E_q^0(\ell) \equiv \int d\ell \eta_q(\ell) = -\frac{1}{16} \ln \left(\frac{\cosh(4\tilde{\omega}_q^2 \ell + C_q) - 1}{\cosh(4\tilde{\omega}_q^2 \ell + C_q) + 1} \right) \tag{2.41}$$

We can now determine the explicit ℓ-dependence of the parameters ω_q and v_q from Eq. (2.38) if we rewrite the set in the following form: $\partial_\ell \omega_q = 8\eta_q v_q$, $\partial_\ell v_q = 2\eta_q \omega_q$. We obtain the following solution:

$$\omega_q(\ell) = \cosh(4E_q(\ell))\omega_q^0 + \sinh(4E_q(\ell))2v_q^0 \tag{2.42}$$
$$v_q(\ell) = (\cosh(4E_q(\ell))2v_q^0 + \sinh(4E_q(\ell))\omega_q^0)/2 \quad , \tag{2.43}$$

where we defined $E_q(\ell) \equiv \int_0^\ell d\ell' \eta_q(\ell')$. One can convince oneself that these solutions indeed yield the correct boundary values for $\ell \to \infty$.

Since $[\eta(\ell), \eta(\ell')] = 0$ we can also calculate the unitary operator U that diagonalizes the TL Hamiltonian. Generally it is given by $U = U(\ell = \infty)$ with $U(\ell) = L\exp(\int_0^\ell d\ell' \eta(\ell'))$. The operator L denotes the ℓ-ordering operator, defined in the same way as the more familiar time-ordering operator

T. We obtain $U = \exp(\sum_{q\neq 0} E_q^*(b_q b_{-q} - b_{-q}^\dagger b_q^\dagger))$ with the familiar relation $\tanh(4E_q^*) = -v_q/(2\pi v_F + v_q)$, where we defined $E_q^* \equiv E_q(\ell = \infty)$.

To determine the flow of the observables we will use the "bosonic" representation of the one-dimensional fermionic field operator of the left- and right-movers $\psi^{L/R}(x)$ which involves the operators of the bosonic density-fluctuation , see e.g. Ref. [Hal81]. It is given by $\psi^{L/R}(x) = F^{L/R}(x)e^{\phi^{L/R}(x)}$, where the operator $F^{L/R}(x)$ lowers the number of left- and right-movers by one respectively and commutes with the bosonic operators $b_q^{(\dagger)}$, i.e. $[b_q^{(\dagger)}, F^{L/R}(x)] = 0$. The phase field is defined as

$$\phi^{L/R}(x) \equiv \sum_{q>0} n_q^{-1/2}(b_{\mp q}e^{\mp iqx} - b_{\mp q}^\dagger e^{\pm iqx}) \quad , \tag{2.44}$$

where, for convenience, we omitted the ultraviolet convergence factor, formally necessary in the case of the non-normal ordered representation of $\psi^{L/R}(x)$. This will not affect the validity of the calculations. Further, we will confine ourselves to the transformation of the field of the right-movers, since the calculations are analogous in the case of the left-movers.

Let U denote the unitary transformation that diagonalizes the TL Hamiltonian of Eq. (2.33). Then $U\psi^R(x)U^\dagger = F^R(x)e^{U\phi^R(x)U^\dagger}$ since U only consists of bosonic operators and thus commutes with $F^R(x)$. Therefore it suffices to consider the Flow Equations for $\phi^R(x)$, i.e. $\partial_\ell \phi^R(x) = [\eta, \phi^R(x)]$. During the flow of $\phi^R(x) \equiv \sum_{q>0} \phi_q^R(x,\ell)$ different wave numbers do not couple and we are allowed to limit ourself to the flow of $\phi_q^R(x,\ell) = \varphi_q^R(\ell)\phi_q^R(x) + \varphi_q^L(\ell)\phi_q^L(x)$, with $\phi_q^{L/R}(x) \equiv b_{\mp q}e^{\mp iqx} - b_{\mp q}^\dagger e^{\pm iqx}$. This yields the following Flow Equations:

$$\partial_\ell \varphi_q^R = -2\eta_q \varphi_q^L \quad , \quad \partial_\ell \varphi_q^L = -2\eta_q \varphi_q^R \tag{2.45}$$

With the initial conditions $\varphi_q^R(\ell = 0) = n_q^{-1/2}$ and $\varphi_q^L(\ell = 0) = 0$ this yields the following solution:

$$\varphi_q^R(\ell) = n_q^{-1/2}\cosh(2E_q(\ell)) \quad , \quad \varphi_q^L(\ell) = -n_q^{-1/2}\sinh(2E_q(\ell)) \tag{2.46}$$

In the limit $\ell \to \infty$ we recover the well-known result for the transformed field operator

$$\psi^R(x) \to F^R(x)\exp\Big(\sum_{q>0}\big(\frac{c_q}{\sqrt{n_q}}(b_q e^{iqx} - b_q^\dagger e^{-iqx}) - \frac{s_q}{\sqrt{n_q}}(b_{-q}e^{-iqx} - b_{-q}^\dagger e^{iqx})\big)\Big) \quad , \tag{2.47}$$

with $c_q \equiv \cosh(2E_q^*)$, $s_q \equiv \sinh(2E_q^*)$, and $s_q^2 = (\omega_q^0/\tilde{\omega}_q - 1)/2$, see e.g. Ref. [Sch97]. The Flow Equations thus yield the same result as applying the Bogoljubov transformation. Correlation functions in position-time space are now easily calculated.

2.2.3. Approximations

It is not surprising that the Flow Equation approach could be applied in a rather straightforward manner since again we took advantage of the bosonization technique. Now we want to calculate the commutator $[\eta, \psi^R(x)]$ directly, employing the usual representation $\psi^R(x) = L^{-1/2} \sum_k e^{ikx} c_k^R$. With the commutator relation

$$[b_q + b_q^\dagger, \psi^R(x)] = -\Theta(q) n_q^{-1/2} (e^{-iqx} + e^{iqx}) \psi^R(x) \quad , \tag{2.48}$$

we obtain:

$$[\eta, \psi^R(x)] = -2 \sum_{q>0} \eta_q n_q^{-1/2} (b_{-q} e^{-iqx} - b_{-q}^\dagger e^{iqx}) \psi^R(x) \tag{2.49}$$

Further we have $[\eta, \phi_q^{L/R}(x)] = -2\eta_q \phi_q^{R/L}(x)$. The Flow Equations thus do not close but generate an infinite series of operators. In the following we only want to consider the terms linear in the fields $\phi_q^{L/R}(x)$. We thus make the following ansatz for the fermionic field:

$$\psi^R(x, \ell) = \psi^R(x) \big(g(\ell) + \sum_{q>0} \varphi_q^R(\ell) \phi_q^R(x) + \varphi_q^L(\ell) \phi_q^L(x) \big) \quad , \tag{2.50}$$

with the initial conditions $g(\ell = 0) = 1$ and $\varphi_q^{L/R}(\ell = 0) = 0$. Notice that $[\psi^R(x), \phi^{L/R}(x)] = 0$.

The Flow Equations depend on the truncation scheme. If one simply cuts the series after the linear term, the parameter g is left un-renormalized, i.e. $g = 1$ for all ℓ. The Flow Equations for the parameters of the terms linear in the bosonic operators then read

$$\partial_\ell \varphi_q^R = -2\eta_q \varphi_q^L \quad , \quad \partial_\ell \varphi_q^L = -2\eta_q \varphi_q^R - 2n_q^{-1/2} \eta_q \quad . \tag{2.51}$$

An analytic solution is now possible: Let $\varphi_q^{hom}(\ell) \equiv e^{-2\sigma_x E_q^0(\ell)}$, then $\vec{\varphi}_q(\ell) = \varphi_q^{hom}(\ell) \vec{\xi}_q(\ell)$ with $\vec{\xi}_q(\ell) = \int_0^\ell d\ell' (\varphi_q^{hom}(\ell'))^{-1} \vec{u}_q(\ell')$, where we defined $\vec{\varphi}_q \equiv (\varphi_q^R, \varphi_q^L)^T$ and $\vec{u}_q \equiv (0, -2n_q^{-1/2} \eta_q)^T$ and σ_x denotes the x-component of the Pauli spin matrices. With the definite integral

$$2 \int_0^\ell d\ell' \eta(\ell') e^{\pm 2E_q^0(\ell')} = \pm (e^{\pm 2E_q^0(\ell)} - e^{\pm 2E_q^0(0)}) \tag{2.52}$$

this yields the following solution:

$$\vec{\xi}_q(\ell) = -n_q^{-1/2} \begin{pmatrix} \cosh(2E_q^0(\ell)) - \cosh(2E_q^0(\ell = 0)) \\ \sinh(2E_q^0(\ell)) - \sinh(2E_q^0(\ell = 0)) \end{pmatrix} \tag{2.53}$$

In the limit $\ell \to \infty$ we obtain with $E_q^0(\ell = 0) = -E_q^*$ the final result

$$\varphi_q^R(\ell = \infty) = n_q^{-1/2} (c_q - 1) \quad , \quad \varphi_q^L(\ell = \infty) = -n_q^{-1/2} s_q \quad . \tag{2.54}$$

Expanding also the fermionic field up to linear bosonic operators, i.e. $\psi^R(x) \to F^R(x)(1+\sum_{q>0} n_q^{-1/2}\phi_q^R(x))$, we see that the Flow Equation approach yields the correct result up to terms which are linear in the bosonic operators, i.e. $U\psi^R(x)U^\dagger \to F^R(x)(1+\sum_{q>0} n_q^{-1/2}(c_q\phi_q^R(x) - s_q\phi_q^L(x))$. This is *not* a perturbative result since the "Bogoljubov-coefficients" s_q and c_q are exactly recovered.

We will come back to transformed field operator later. Before we will transform the fermionic ladder operators of the right-movers c_k^R. The Flow Equations create an infinite series; we will therefore again truncate the series after the terms which are linear in the bosonic operators:

$$c_k^R(\ell) = g(\ell)c_k^R + \sum_{q>0}(\varphi_q^R(\ell)\phi_{q,k}^R + \varphi_q^L(\ell)\phi_{q,k}^L) \quad , \tag{2.55}$$

with the initial conditions $g(\ell=0)=1$ and $\varphi_q^{L/R}(\ell=0)=0$ and where we defined $\phi_{q,k}^{L/R} \equiv (b_{\mp q}c_{k\pm q}^R - b_{\mp q}^\dagger c_{k\mp q}^R)$.

Neglecting terms which are bilinear in the bosonic operators and in their non-normal ordered form leads to the same differential equations as for the flow parameters of the truncated fermionic field operator, given in Eq. (2.50). The solution is thus again given by $g=1$ for all ℓ and

$$\varphi_q^R(\ell=\infty) = n_q^{-1/2}\tilde{c}_q \quad , \quad \varphi_q^L(\ell=\infty) = -n_q^{-1/2}s_q \quad , \tag{2.56}$$

where we abbreviated $\tilde{c}_q \equiv c_q - 1$.

So far we do not know what effect the truncation scheme of Eq. (2.55) has got on physical quantities. For this reason it is useful to calculate the occupation function in momentum space in this approximation, i.e. $n_k^{R,1} \equiv \langle FDS|c_k^{R\dagger}(\ell=\infty)c_k^R(\ell=\infty)|FDS\rangle$, where $|FDS\rangle$ denotes the ground-state of the Fermi-Dirac sea. We obtain the following result:

$$\begin{aligned} n_k^{R,1} &= (1-\sum_{q>0}\frac{\tilde{c}_q}{n_q})^2\Theta(k_F-k) + 2(1-\sum_{q>0}\frac{\tilde{c}_q}{n_q})\sum_{q>0}\frac{\tilde{c}_q}{n_q}\Theta(k_F-q-k) \\ &+ \sum_{q>0}\frac{\tilde{c}_q}{n_q}\sum_{q'>0}\frac{\tilde{c}_{q'}}{n_{q'}}\Theta(k_F-q-q'-k) \\ &+ \sum_{q>0}\frac{\tilde{c}_q^2}{n_q}\Theta(k_F-q-k) + \sum_{q>0}\frac{s_q^2}{n_q}\Theta(k_F+q-k) \quad , \end{aligned} \tag{2.57}$$

with the step function $\Theta(k)$ which equals one for $k \geq 0$ and zero otherwise.

Considering $k = k_F + \tilde{q}$ with $\tilde{q} > 0$ only the last term of Eq. (2.57) contributes to $n_k^{R,1}$. It is now convenient to work with a finite interaction cutoff $q_c \equiv 2\pi n_c/L$ and choose the interaction potential as a step function in momentum space, i.e. $s_q = s$ for $q \leq q_c$ and $s_q = 0$ for $q > q_c$. With $\sum_{n=1}^{n_c} 1/n \to \ln n_c + C$ for $n_c \to \infty$, where $C = 0.57721...$ is Euler's constant we find in the thermodynamic limit $L \to \infty$, $N/L = \text{const}$ the following expression:

$$n^{R,1}_{k_F+\tilde{q}} = \sum_{q>0} \frac{s_q^2}{n_q} \Theta(k_F + q - k) \to -s^2 \ln(\tilde{q}/q_c) \to (1 - (\tilde{q}/q_c)^{2s^2})/2 \tag{2.58}$$

The last limit was taken in the case of weak coupling, i.e $s^2 \ll 1$. In this perturbative regime we thus recover the well-known power law behaviour around the Fermi point k_F; and we observe the peculiar situation that the truncation scheme of Eq. (2.55) yields the *exact* anomalous dimension $\alpha \equiv 2s^2$, see e.g. Ref. [Sch97].

For wave numbers below the Fermi point, i.e. for $k = k_F - \tilde{q}$ with $\tilde{q} > 0$, the calculations are not so plane. But if we simply neglect $\sum_{q,q'>0} \tilde{c}_q \tilde{c}_{q'}/(n_q n_{q'})(\Theta(k_F + q - k)\Theta(k_F + q' - k) + \Theta(k_F - q - q' - k) - \Theta(k_F - q - k)\Theta(k_F - q' - k))$ and $\sum_{q>0}(\tilde{c}_q^2 + s_q^2)/n_q$, one obtains for the whole regime in the limit of small coupling

$$n^{R,1}_{k_F+\tilde{q}} = 1/2 - \text{sgn}(\tilde{q})/2(|\tilde{q}|/q_c)^{\alpha} \quad . \tag{2.59}$$

The pre-factor 1/2 in front of the power-law behaviour is also recovered from simple perturbation theory [Sch97]. This factor could not be recovered unambiguously from the calculations of the approximate occupation number of the n-orbital model [Weg94].

Finally we want to check if also dynamic quantities can be recovered from the truncation scheme of Eq. (2.50). For this we will calculate the approximate Green function defined as

$$iG_R^{<,1}(x,t) \equiv \langle FDS|\psi^{R^\dagger}(x=0,\ell=\infty)e^{iH_\infty t}\psi^R(x,\ell=\infty)e^{-iH_\infty t}|FDS\rangle \quad , \tag{2.60}$$

with $H_\infty \equiv H(\ell = \infty)$.

In order to evaluate the time dependence of the fermionic field of the right-movers we have to work with a constant potential in momentum space, i.e. $v_q = v$. This yields a linear energy dispersion for the fixpoint Hamiltonian, i.e. $H_\infty = v_c \sum_{q\neq 0} |q| b_q^\dagger b_q$ with the renormalized Fermi velocity or charge velocity $v_c \equiv v_F(1 + v/(\pi v_F))^{1/2}$. With the help of the Kronig relation of Eq. (2.32) and again neglecting terms that include the number-of-particle operator of the left- and right-movers, the time dependence of the fermionic and bosonic ladder operators in the Heisenberg representation at $\ell = \infty$ are given by $c_k(t) = c_k e^{-ikv_c t}$ and $b_q(t) = b_q e^{-i|q|v_c t}$.

The Green function of Eq. (2.60) can now be expressed as a function of the conformal variables $\xi^{L/R} \equiv x \pm v_c t$ and yields

$$\begin{aligned} iG_R^{<,1}(\xi^R,\xi^L) &= iG_R^{<,0}(\xi^R) \\ &\times \Big((1 - \sum_{q>0} \frac{\tilde{c}_q}{n_q}(1 - e^{-iq\xi^R}))^2 + \sum_{q>0} \frac{\tilde{c}_q^2}{n_q} e^{-iq\xi^R} + \sum_{q>0} \frac{s_q^2}{n_q} e^{iq\xi^L} \Big) \quad , \end{aligned} \tag{2.61}$$

with $iG_R^{<,0}(\xi^R) \equiv \langle FDS|\psi^{R\dagger}(x=0,\ell=0)e^{iH_\infty t}\psi^R(x,\ell=0)e^{-iH_\infty t}|FDS\rangle = L^{-1}\sum_k e^{ik\xi^R}\Theta(k_F-k)$.

An important consistency check of the truncation schemes in Eqs. (2.50) and (2.55) is given by the fact that $n_k^{R,1} = \int_{-L/2}^{L/2} dx e^{-ikx} iG_R^{<,1}(x,t=0)$. But working with a constant potential in momentum space, i.e. a delta-potential in position space, yields the well-known ultraviolet divergences. In the following we will therefore introduce an ultraviolet cutoff and also label it with q_c.

A physical observable is given by the occupied density of states $\rho_R^<(\omega)$ which is observed in photoemission experiments. Based on the exact Green function $G_R^<(x,t)$ it is defined as

$$\rho_R^<(\omega) \equiv \frac{1}{2\pi}\int dt e^{i\omega t} iG_R^<(x=0,t) \quad . \tag{2.62}$$

Inserting the approximated Green function $G_R^{<,1}(x=0,t)$ yields with $\omega = v_c k_F - \tilde{\omega}$

$$\begin{aligned}\rho_R^{<,1}(\tilde{\omega}) = \frac{\Theta(\tilde{\omega})}{2\pi v_c}\Big((1 &- \sum_{q>0}\frac{\tilde{c}_q}{n_q} + \sum_{q>0}\frac{\tilde{c}_q}{n_q}\Theta(\tilde{\omega}-v_c q))^2 \\ &+ \sum_{q,q'>0}\frac{\tilde{c}_q}{n_q}\frac{\tilde{c}_{q'}}{n_{q'}}(\Theta(\tilde{\omega}-v_c(q+q')) - \Theta(\tilde{\omega}-v_c q)\Theta(\tilde{\omega}-v_c q')) \\ &+ \sum_{q>0}\frac{\tilde{c}_q^2}{n_q}\Theta(\tilde{\omega}-v_c q) + \sum_{q>0}\frac{s_q^2}{n_q}\Theta(\tilde{\omega}-v_c q)\Big)\end{aligned} \tag{2.63}$$

Neglecting the same terms as in the case of the calculation of the occupation number, i.e. $\sum_{q,q'>0}\tilde{c}_q\tilde{c}_{q'}/(n_q n_{q'})(\Theta(v_c q-\tilde{\omega})\Theta(v_c q'-\tilde{\omega}) + \Theta(\tilde{\omega}-v_c(q+q')) - \Theta(\tilde{\omega}-v_c q)\Theta(\tilde{\omega}-v_c q'))$ and $\sum_{q>0}(\tilde{c}_q^2+s_q^2)/n_q$, we obtain in the thermodynamic limit $\rho_R^{<,1}(\tilde{\omega}) = \Theta(\tilde{\omega})(1+2s^2\ln(\tilde{\omega}/(v_c q_c))/(2\pi v_c)$. In the limit of small coupling we thus obtain the well-known algebraic suppression at the renormalized Fermi energy, again governed by the *exact* anomalous dimension $\alpha = 2s^2$:

$$\rho_R^{<,1}(v_c k_F - \tilde{\omega}) = \frac{\Theta(\tilde{\omega})}{2\pi v_c}\left(\frac{\tilde{\omega}}{v_c q_c}\right)^\alpha \tag{2.64}$$

The *exact* spectral function for a step function potential with cutoff q_c is only modified by the factor $e^{-\alpha C}/\Gamma(1+\alpha)$, with C denoting Euler's constant and $\Gamma(x)$ Euler's Gamma function [Sch97]. Furthermore, we want to note that for the static correlation function $n_k^{R,1}$ the anomalous dimension is being accounted for by either left-movers ($k > k_F$) or right-movers ($k > k_F$) whereas both branches contribute to the anomalous dimension in equal parts in case of the dynamic correlation function $\rho_R^{<,1}$.

These two examples show that the Flow Equation approach can yield exact, non-perturbative results even within a rather crude truncation scheme. This observation can be useful for non-exactly solvable model, e.g. if one adds an impurity $H_i = \lambda\psi^\dagger(x = 0)\psi(x = 0)$ to the TL Hamiltonian given in Eq. (2.33), see e.g. Ref. [Kan92]. The transport properties in the latter model are directly related to the transport properties of a Brownian particle in a tilted cosine potential [Wei99]. We will consider this model in Chapter 5.

2.3. Dissipative Harmonic Oscillator

We will now turn to dissipative systems. Since the method we want to use is based on the Hamiltonian formulation we will adopt the well established standpoint to describe both, system and bath, as an isolated system. Dissipation enters through the fact that once energy has been transferred from the system to the infinite bath it will take an infinite amount of time until it will be transferred back to the system and has thus dissipated.

Following the seminal work by Caldeira and Leggett [Cal83], we will model the bath as a set of non-interacting harmonic oscillators with a dense spectrum. We will also introduce the interaction induced renormalization of the potential so that the Hamiltonian is bounded from below.

The Dissipative Harmonic Oscillator is thus given by the following Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sigma v \hat{q}^2 + \sum_\alpha \left(\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{1}{2} m_\alpha \omega_\alpha^2 (\hat{x}_\alpha - \frac{\lambda_\alpha}{m_\alpha \omega_\alpha^2} \hat{q})^2 \right) + E \tag{2.65}$$

The operators are denoted by a hat which shall be dropped from now on. They obey the canonical commutation relations which read

$$[q, p] = i \quad , \quad [x_\alpha, p_{\alpha'}] = i\delta_{\alpha,\alpha'} \quad . \tag{2.66}$$

The parameter σ can be decomposed as $\sigma = V_0/q_0^2$ and we identify the frequency of the harmonic oscillator as $\omega_0^2 = 2V_0 v/mq_0^2$. The notation has been chosen so that it can be easily compared with the dissipative system of a particle in a periodic potential discussed in Chapter 5.

Expressing the partition function of the canonical ensemble $Z = \langle e^{-\beta H} \rangle$ in terms of path integrals, the exact solvability of the model enters through the fact that only Gaussian integrals are involved. For other models, e.g. the Spin-Boson Model, approximations become necessary. The most prominent is given by the Non-Interacting Blip Approximation (NIBA) which is a perturbative treatment of the tunnel-matrix element based on the functional integral representation of the model [Leg87]. Nevertheless it fails in the description of the system dynamics on *all* time scales.

The exact solution of the model, following the Flow Equation approach, is less obvious and was first obtained by Kehrein and Mielke [Keh97]. The big advantage though is that it can be generalized to non-trivial models, like the Spin-Boson Model, and still keep its validity over all time or energy scales. This is an essential feature of renormalization schemes. We will therefore recall the solution of Kehrein and Mielke briefly in this section and also extend the solution to more universal results.

2.3.1. Analytical Results

In order to solve the Dissipative Harmonic Oscillator via Flow Equations, the generator η of the infinitesimal unitary transformations is chosen to be

$$\eta = i\Big(q\sum_\alpha \eta^q_\alpha p_\alpha + p\sum_\alpha \eta^p_\alpha x_\alpha + \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'} x_\alpha p_{\alpha'}\Big) \equiv \eta^q + \eta^p + \eta_B \quad . \tag{2.67}$$

The first two terms follow from the canonical choice $\eta = [H_0, V]$ with the off-diagonal part $V = -q\sum_\alpha \lambda_\alpha x_\alpha$, but with generalized parameters η^q_α and η^p_α. They will be determined later. The last term η^B is needed to cancel a new interaction term between the different bath modes which is generated by the Flow Equations. The exact solvability of the model enters through the fact that this cancellation is exact and that therefore the Flow Equations close exactly.

The commutator $[\eta, H]$ yields the following contributions:

$$[\eta^q, H] = -p\sum_\alpha \eta^q_\alpha \frac{p_\alpha}{m} + q\sum_\alpha \eta^q_\alpha m_\alpha \omega^2_\alpha (x_\alpha - \frac{\lambda_\alpha}{m_\alpha \omega^2_\alpha} q) \tag{2.68}$$

$$[\eta^p, H] = 2\sigma v q \sum_\alpha \eta^p_\alpha x_\alpha - p\sum_\alpha \eta^p_\alpha \frac{p_\alpha}{m_\alpha} - \sum_{\alpha,\alpha'} \eta^p_\alpha x_\alpha \lambda_{\alpha'} (x_{\alpha'} - \frac{\lambda_{\alpha'}}{m_{\alpha'}} q) \tag{2.69}$$

$$[\eta_B, H] = -\sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'} \frac{p_\alpha p_{\alpha'}}{m_\alpha} + \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'} x_\alpha m_{\alpha'} \omega^2_{\alpha'} (x_{\alpha'} - \frac{\lambda_{\alpha'}}{m_{\alpha'}\omega^2_{\alpha'}} q) \tag{2.70}$$

The constants of the generator are now chosen in such a way that the Hamiltonian remains form-invariant during the flow, i. e. that no new interaction terms are generated. This leads to the following relations:

$$\eta^q_\alpha m_\alpha + \eta^p_\alpha m = 0 \tag{2.71}$$

$$\eta_{\alpha,\alpha'} m_{\alpha'} + \eta_{\alpha',\alpha} m_\alpha = 0 \tag{2.72}$$

$$\eta_{\alpha,\alpha'} m_{\alpha'} \omega^2_{\alpha'} + \eta_{\alpha',\alpha} m_\alpha \omega^2_\alpha - (\eta^p_\alpha \lambda_{\alpha'} + \eta^p_{\alpha'} \lambda_\alpha) = 0 \tag{2.73}$$

Eqs. (2.72) and (2.73) make sure that the bilinear terms in the bath operators vanish, i.e. $: p_\alpha p_{\alpha'} :$ and $: x_\alpha x_{\alpha'} :$, where $: ... :$ denotes normal ordering with respect to the free bath. Normal ordering is necessary in order to deal with well-defined quantities and by $\langle x^2_\alpha \rangle = (1 + 2n_\alpha)/(2m_\alpha \omega_\alpha)$ a shift in the energy is induced, $n_\alpha \equiv (e^{\beta\omega_\alpha} - 1)^{-1}$ denoting the Bose factor. The Flow Equations are given by

$$\begin{aligned} \partial_\ell \tilde{v} &= -\sigma^{-1}\sum_\alpha \eta^q_\alpha \lambda_\alpha \quad , \quad \partial_\ell E = -\sum_\alpha \eta_\alpha \lambda_\alpha \langle x^2_\alpha \rangle \\ \partial_\ell \lambda_\alpha &= -\eta^q_\alpha m_\alpha \omega^2_\alpha - \eta^p_\alpha \sigma 2\tilde{v} + \sum_{\alpha'} \eta_{\alpha,\alpha'} \lambda_{\alpha'} \quad , \end{aligned} \tag{2.74}$$

with the renormalized potential $\tilde{v} \equiv v + \sigma^{-1}\sum_\alpha \frac{\lambda^2_\alpha}{2m_\alpha \omega^2_\alpha}$. Notice that renormalization of the bath modes ω_α are already neglected since they vanish in the thermodynamic limit.

Parameterizing the constants as follows

$$\eta^p_\alpha = \lambda_\alpha f(\omega_\alpha,\ell)/m \tag{2.75}$$
$$\eta^q_\alpha = -\lambda_\alpha f(\omega_\alpha,\ell)/m_\alpha \tag{2.76}$$
$$\eta_{\alpha,\alpha'} = -\lambda_\alpha\lambda_{\alpha'}(f(\omega_\alpha,\ell)+f(\omega_{\alpha'},\ell))/(\omega^2_\alpha-\omega^2_{\alpha'})/(m_{\alpha'}m) \tag{2.77}$$

and introducing the spectral function

$$J(\omega,\ell) = \sum_\alpha \frac{\lambda^2_\alpha}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha) \quad , \tag{2.78}$$

the following coupled integro-differential equations are obtained:

$$\partial_\ell\tilde{v} = \sigma^{-1}\int d\omega J(\omega,\ell)\omega f(\omega,\ell) \tag{2.79}$$
$$\partial_\ell E = -\frac{1}{2m}\int d\omega J(\omega,\ell)f(\omega,\ell)(1+2n(\omega)) \tag{2.80}$$
$$\begin{aligned}\partial_\ell J(\omega,\ell) &= 2J(\omega,\ell)\omega^2 f(\omega,\ell) - 4\frac{\tilde{v}}{m}\sigma J(\omega,\ell)f(\omega,\ell) \\ &\quad - \frac{2}{m}J(\omega,\ell)\int d\omega'\frac{J(\omega',\ell)\omega'}{\omega^2-\omega'^2}(f(\omega,\ell)+f(\omega',\ell))\end{aligned} \tag{2.81}$$

Notice that there is no mass renormalization in this approach. The above Flow Equations are equivalent to the ones obtained by Kehrein and Mielke if one identifies $\Delta^2_{KM} = 2\sigma\tilde{v}/m$ and $4\Delta_{KM}J_{KM}(\omega,\ell) = J(\omega,\ell)/m$, where we added the subscript KM on their notations [Keh97].

To solve these equations Mielke and Kehrein introduced the function

$$R(z,\ell) = \sum_\alpha \frac{\lambda^2_\alpha}{m_\alpha(z-\omega^2_\alpha)} \quad , \tag{2.82}$$

for which the following differential equation holds:

$$\partial_\ell R(z,\ell) = -2\sigma\partial_\ell\tilde{v} + 2(mz-2\sigma\tilde{v}-R(z,\ell))\sum_\alpha\frac{\lambda^2_\alpha}{m_\alpha m(z-\omega^2_\alpha)}f(\omega_\alpha,\ell) \tag{2.83}$$

The algebraic equation $mz - 2\sigma\tilde{v} - R(z,\ell) = 0$ solves the differential equation (2.83) for any z. With $mz^* = 2\sigma\tilde{v}(\ell=\infty)$ one imposes the boundary condition $R(z^*,\ell)\to 0$ for $\ell\to\infty$ which guarantees that system and bath are decoupled for $\ell\to\infty$. This yields a self-consistent equation for $\tilde{v}(\ell=\infty)$ which can at least formally be solved by setting $\ell=0$ and by inserting the initial conditions for the system and coupling parameters. Generally it reads

$$\omega^2_\infty = \omega^2(\ell) + \frac{1}{m}\int d\omega\frac{J(\omega,\ell)\omega}{\omega^2_\infty-\omega^2} \quad , \tag{2.84}$$

where we introduced the ℓ-dependent frequency of the dissipative harmonic oscillator $\omega^2(\ell) \equiv 2\sigma\tilde{v}(\ell)/m$ and $\omega_\infty \equiv \omega(\ell = \infty)$. We want to mention that for this reasoning ω_∞ has to be finite, i.e. $\tilde{v}(\ell = \infty) > 0$. Otherwise the two boundary conditions $R(z^*, \ell = \infty) = 0$ and Eq. (2.84) at $\ell = 0$ cannot be satisfied unless $v(\ell = 0) = 0$. The latter case describes the system of a dissipative free particle.

To determine correlation functions we have to apply the same sequence of infinitesimal transformations to the observables that led to the diagonalization of the Hamiltonian. Only then the diagonal structure of the Hamiltonian can be used to yield a simple time evolution of the operators in the Heisenberg representation. For the flow of the position operator we make the ansatz

$$q(\ell) = h(\ell)q + \sum_\alpha \chi_\alpha(\ell)x_\alpha \quad . \tag{2.85}$$

The initial conditions are given by $h(\ell = 0) = 1$ and $\chi_\alpha(\ell = 0) = 0$. During the flow, the weight of the system operator will be transferred to the bath operators. In the language of the Flow Equation approach we speak of a dissipative system when the total weight of the system is being transferred to the bath during the flow, i.e. $h(\ell = \infty) = 0$.

The Flow Equations for the observable $\partial_\ell q = [\eta, q]$ close and we obtain:

$$\partial_\ell h = \sum_\alpha \eta^q_\alpha \chi_\alpha = -\sum_\alpha \frac{\lambda_\alpha \chi_\alpha}{m_\alpha} f(\omega_\alpha, \ell) \tag{2.86}$$

$$\begin{aligned} \partial_\ell \chi_\alpha &= h\eta^p_\alpha + \sum_{\alpha'} \eta_{\alpha,\alpha'}\chi_{\alpha'} \\ &= h\frac{\lambda_\alpha}{m} f(\omega_\alpha, \ell) - \lambda_\alpha \sum_{\alpha'} \frac{\lambda_\alpha \chi_\alpha}{\omega_\alpha^2 - \omega_{\alpha'}^2} \frac{1}{m_{\alpha'} m} (f(\omega_\alpha, \ell) + f(\omega_{\alpha'}, \ell)) \end{aligned} \tag{2.87}$$

The Flow Equations for $p(\ell) = h(\ell)p + \sum_\alpha \chi_\alpha(\ell)p_\alpha$ are obtained from the above Flow Equations by interchanging $\eta^p_\alpha \to -\eta^q_\alpha$ and $\eta^q_\alpha \to -\eta^p_\alpha$. According to Eq. (2.71), η^p_α and η^q_α only differ by a sign and a constant since there is no mass renormalization. Thus the Flow Equations of the observables $q(\ell)$ and $p(\ell)$ are equivalent which means that Hermite-city is conserved during the flow.

From these Flow Equations we obtain the following sum rule, which expresses the fact that the commutation relation $[q, p] = i$ holds for all ℓ:

$$h^2 + m\sum_\alpha \frac{\chi_\alpha^2}{m_\alpha} = 1 \tag{2.88}$$

To solve the Flow Equations one introduces the functions

$$S_1(z, \ell) = \sum_\alpha \frac{\lambda_\alpha \chi_\alpha}{m_\alpha(z - \omega_\alpha^2)} \quad , \quad S_2(z, \ell) = \sum_\alpha \frac{\chi_\alpha^2}{m_\alpha(z - \omega_\alpha^2)} \quad . \tag{2.89}$$

Mielke and Kehrein showed that the following quantity is conserved:

$$S_2(z,\ell) + \frac{(h(\ell) - S_1(z,\ell))^2}{mz - 2\sigma\tilde{v}(\ell) - R(z,\ell)} = \text{const.} \tag{2.90}$$

Thus one ends up with

$$S_2(z,\ell=\infty) + \frac{h(\ell=\infty)^2}{mz - 2\sigma\tilde{v}(\ell=\infty)} = (mz - 2\sigma\tilde{v}(\ell=0) - R(z,\ell=0))^{-1} \quad . \tag{2.91}$$

Comparing the pole structure of both sides of Eq. (2.91) one sees that $h(\ell=\infty)=0$ for the initial conditions of interest. This shows that indeed all the total weight of the system is being transferred to the system. The particle has dissipated.

Correlation functions are obtained through the following identity:

$$K(\omega,\ell) \equiv \sum_\alpha \frac{\chi_\alpha(\ell)^2}{m_\alpha}\delta(\omega^2 - \omega_\alpha^2) = \frac{1}{\pi}\mathrm{Im}S_2(\omega^2 - i0,\ell) \tag{2.92}$$

For example, the spectral function $\omega K(\omega) \equiv \omega K(\omega,\ell=\infty)$ is proportional to the Fourier transform of $\langle q(t)q\rangle$, where $\langle ...\rangle$ denotes the ground-state expectation value and the time evolution is governed by the full Hamiltonian H. Extensions to finite temperatures are straightforward [Keh97].

Choosing a Lorentzian spectral function

$$J(\omega) \equiv J(\omega,\ell=0) = \frac{4\gamma^2\omega\alpha}{\gamma^2+\omega^2} \quad , \tag{2.93}$$

the explicit solution follows from Eq. (2.91) ($\omega_0 \equiv \omega(\ell=0)$):

$$K(\omega) = \frac{2\alpha\gamma^2\omega_0\omega(\gamma^2+\omega^2)}{(\omega_0^2(\gamma^2+\omega^2) - 2\pi\alpha\gamma^3\omega_0 - \omega^2(\gamma^2+\omega^2))^2 + 4\pi^2\alpha^2\omega_0^2\gamma^4\omega^2} \tag{2.94}$$

2.3.2. Universal Asymptotic Behaviour

It is often useful to explicitly specify the function $f(\omega,\ell)$ even though the final result must be independent of the particular choice. In a slightly different context Kehrein, Mielke, and Neu chose $f(\omega,\ell) = -(\omega-\omega(\ell))/(\omega+\omega(\ell))$ [Keh96b]. This leads to $J(\omega,\ell) \propto \exp(-2(\omega-\omega(\ell))^2\ell)$ for $\ell\to\infty$ if one neglects the non-linear term of $J(\omega,\ell)$ in Eq. (2.81). The spectral function is therefore centered around the renormalized frequency ω_∞, defined in Eq. (2.84). At $\omega=\omega_\infty$ the spectral function vanishes algebraically as $\ell^{-1/2}$. The asymptotic spectral function thus depends on the initial frequency through ω_∞. We want to label this asymptotic behaviour *non-universal*.

A different choice is $f(\omega,\ell) = -1$ which would have the consequence that the renormalized potential has to tend to zero so that the system is decoupled for $\ell\to\infty$, i.e. $\tilde{v}(\ell=\infty)=0$ in order that $J(\omega,\ell=\infty)=0$. It therefore belongs to a different universality class since Eq. (2.84) does not hold anymore. The Differential Equation (2.83) turns into a Ricatti-Equation which can be formally integrated. For $z = 0$ this yields:

$$R(z=0,\ell) = 2\sigma\left(\frac{v(\ell=0)}{u_{\text{inh}}(\ell)} - \tilde{v}(\ell)\right) \quad \text{, with} \tag{2.95}$$

$$u_{\text{inh}}(\ell) = u_{\text{hom}}(\ell)\left(1 - \frac{2}{m}\int_0^\ell d\ell' \frac{2\sigma v(\ell=0)}{u_{\text{hom}}(\ell')}\right) \quad , \quad u_{\text{hom}} = \exp\left(\frac{2}{m}\int_0^\ell d\ell' 2\sigma\tilde{v}(\ell')\right)$$

That the choice $f(\omega,\ell) = -1$ really decouples the system from the bath is not clear from the beginning. One way to convince oneself is to study the asymptotic behaviour of the Flow Equations (2.79) and (2.81). With regard to the Flow Equations of the Spin-Boson Model in Chapter 4 we will consider Flow Equations for slightly different quantities, namely $\Delta(\ell) \equiv \omega(\ell)$ and $\widetilde{J}(\omega,\ell) \equiv J(\omega,\ell)/(m\Delta)$. With $f(\omega,\ell) = -1$ they read

$$\partial_\ell \Delta = -\int d\omega \widetilde{J}(\omega,\ell)\omega \tag{2.96}$$

$$\partial_\ell \widetilde{J}(\omega,\ell) = 2\widetilde{J}(\omega,\ell)(\Delta^2 - \omega^2 - \frac{1}{2\Delta}\partial_\ell\Delta) + 4\Delta\widetilde{J}(\omega,\ell)\int d\omega' \frac{\widetilde{J}(\omega',\ell)\omega'}{\omega^2 - \omega'^2} \tag{2.97}$$

We now make the ansatz $\Delta \to a\ell^{-1/2}$ and $\widetilde{\Lambda}(\ell) \to b\ell^{-1/2}$ with $\widetilde{\Lambda}(\ell) \equiv \int d\omega \widetilde{J}(\omega,\ell)/\omega$ as $\ell \to \infty$. We further parameterize the asymptotic function by one parameter s, i.e. we assume that $\widetilde{J}(\omega,\ell) \to \omega^s \hat{J}(\ell)\bar{J}(y)$, where $y \equiv \omega\sqrt{\ell}$ and $\bar{J}(y) \to J_0$ for $y \to 0$. Notice that we dropped the index s on the functions $\widetilde{J}(\omega,\ell)$, $\hat{J}(\ell)$ and $\bar{J}(y)$.

The differential equation for $\widetilde{\Lambda}$ is given by

$$\partial_\ell \widetilde{\Lambda} = 2\widetilde{\Lambda}(\Delta^2 - \frac{1}{2\Delta}\partial_\ell\Delta) + 2\partial_\ell\Delta - 2\Delta\widetilde{\Lambda}^2 \quad , \tag{2.98}$$

where we used the identity

$$\int d\omega \int d\omega' \frac{\widetilde{J}(\omega)\widetilde{J}(\omega')}{\omega\omega'}\frac{\omega'^2}{\omega^2 - \omega'^2} = -\frac{1}{2}\int d\omega \int d\omega' \frac{\widetilde{J}(\omega)\widetilde{J}(\omega')}{\omega\omega'} \quad . \tag{2.99}$$

The differential equation for $\hat{J}(\ell)$ is obtained from Eq. (2.97) by setting $\omega = 0$. This yields

$$\partial_\ell \hat{J}(\ell) = \hat{J}(\ell)(2\Delta^2 - 4\Delta\widetilde{\Lambda} - \frac{1}{\Delta}\partial_\ell\Delta) \quad . \tag{2.100}$$

Comparing the asymptotic behaviour that follows from the differential equations of $\widetilde{\Lambda}$ and Δ with the above ansatz, one obtains self-consistency if $\hat{J}(\ell) \to \ell^{(s-1)/2}$. From Eq. (2.100) it then follows that $2a^2 - 4ab + 1/2 = (s-1)/2$. From Eq. (2.98) it follows that $-b/2 = 2ba^2 + b/2 - a - 2ab^2$. We thus obtain $a^2 = 1/2 \pm s/4$ and

$b = a(1 - s/4 \pm s/4)/2$. Discussing the asymptotic behaviour of the flow of the observable we will see that one has to choose the plus sign. This also agrees with the numerical results.

With these relations for the constants a and b, we obtain the following non-local differential equation for $J(y) \equiv y^{s-1}\bar{J}(y)$:

$$\partial_y J(y) = -4yJ(y)(1 - 2a\int_0^\infty dy' \frac{J(y')}{y^2 - y'^2}) + (s-1)\frac{J(y)}{y} \tag{2.101}$$

The above ansatz for the asymptotic behaviour guarantees that the system will be decoupled from the bath since the support of the spectral function vanishes as $\ell^{-1/2}$ and $J(y) \to y^{4+(s-1)}e^{-2y^2}$ for $y \to \infty$. There is thus a *universal* fixpoint for all initial frequencies. They are all mapped onto the free particle plus bath. For $y \to 0$, Eq. (2.101) yields $J(y) \to J_0 y^{s-1}$.

We want to investigate the flow of the observable as well. For that we introduce the spectral function

$$S(\omega, \ell) \equiv -\sum_\alpha \frac{\lambda_\alpha \chi_\alpha}{m_\alpha \omega_\alpha}\delta(\omega - \omega_\alpha) \quad . \tag{2.102}$$

With $f(\omega, \ell) = -1$ the Flow Equations (2.86) and (2.87) then read

$$\partial_\ell h = -\int d\omega \omega S(\omega, \ell) \tag{2.103}$$

$$\begin{aligned} \partial_\ell S(\omega, \ell) &= \Delta h J(\omega, \ell) + 2\Delta J(\omega, \ell)\int d\omega' \frac{S(\omega', \ell)\omega'}{\omega^2 - \omega'^2} \\ &+ (\Delta^2 - \omega^2)S(\omega, \ell) + 2\Delta S(\omega, \ell)\int d\omega' \frac{J(\omega', \ell)\omega'}{\omega^2 - \omega'^2} \quad . \end{aligned} \tag{2.104}$$

To determine the asymptotic behaviour of $S(\omega, \ell)$ we make a similar ansatz as in the case of the spectral function $\widetilde{J}(\omega, \ell)$, namely $h(\ell) \to c\ell^{-1/2-\xi}$ and $\Sigma(\ell) \to d\ell^{-1/2-\xi}$ with $\Sigma(\ell) \equiv \int d\omega S(\omega, \ell)/\omega$ as $\ell \to \infty$. Further we assume that $S(\omega, \ell) \to \omega^s \hat{S}(\ell)\bar{S}(y)$, where $y \equiv \omega\sqrt{\ell}$ and $\bar{S}(y) \to S_0$ for $y \to 0$.

The differential equation for Σ is given by

$$\partial_\ell \Sigma = \Delta h \widetilde{\Lambda} + \Delta^2 \Sigma + \partial_\ell h - 2\Delta\widetilde{\Lambda}\Sigma \quad . \tag{2.105}$$

The differential equation for $\hat{S}(\ell)$ is obtained from Eq. (2.104) by setting $\omega = 0$. This yields

$$\partial_\ell \hat{S}(\ell) = \frac{J_0}{S_0}\Delta h - 2\frac{J_0}{S_0}\Delta\Sigma + \frac{1}{2\Delta}\partial_\ell \Delta \hat{S}(\ell) + \frac{s-1}{4}\ell^{-1}\hat{S}(\ell) \quad . \tag{2.106}$$

Comparing the asymptotic behaviour that follows from the differential equations of Σ and h with the above ansatz, one obtains self-consistency if $\hat{S}(\ell) \to \ell^{-\xi+(s-1)/2}$. From

Eq. (2.106) it then follows that $(ac - 2ad)J_0 = -S_0(\xi - s/4) = 0$ for $s \neq 1$. Since the asymptotic behaviour should be independent of the constant S_0 also for $s = 1$ we generally obtain $\xi = s/4$ and $c = 2d$. This is consistent with the differential equation obtained for Σ which reduces to the following algebraic equation in the asymptotic limit: $-(1/2+\xi)d = abc + a^2 d - (1/2+\xi)c - 2abd$ with $ab = 1/2$ and $a^2 = 3/4 + (s-1)/4$.[4]

We obtain the following non-local differential equation for $S(y) \equiv y^{s-1}\bar{S}(y)$:

$$\partial_y S(y) = -2yS(y)(1 - 2a\int_0^\infty dy' \frac{J(y')}{y^2 - y'^2}) + 4ayJ(y)\int_0^\infty dy' \frac{S(y')}{y^2 - y'^2} + (s-1)\frac{S(y)}{y} \tag{2.107}$$

Eq. (2.107) is linear in $S(y)$. We can therefore not determine the constant S_0 from the asymptotic behaviour. The asymptotic solution of Eq. (2.107) yields $S(y) \to S_0 y^{s-1}$ for $y \to 0$ and $S(y) \to y^{2+(s-1)}e^{-y^2}$ for $y \to \infty$. From the relation

$$2mK(\omega, \ell) = \frac{S^2(\omega, \ell)}{\Delta\widetilde{J}\omega, \ell)} \longrightarrow \ell^{-s/2}\frac{y}{a}\frac{S^2(y)}{J(y)} \longrightarrow \ell^{-s/2}\frac{S_0}{J_0}\frac{y^s}{a} \quad , \tag{2.108}$$

where the first limit was for $\ell \to \infty$ and the second limit for either $y \to 0$ or $y \to \infty$, one sees that the asymptotic limits have to be interpreted with care. We will therefore focus on Eq. (2.87) and integrate this equation directly.

Using Eq. (2.87) and for ℓ_1, ℓ_2 both being in the asymptotic regime, we obtain the following relation

$$K(\omega, \ell_2) - K(\omega, \ell_1) = \frac{4}{m}\omega^s \int_{y_1}^{y_2} dy y^{2-s} S(y) \int_0^\infty dy' \frac{S(y')}{y^2 - y'^2} \quad , \tag{2.109}$$

with $y_i = \omega\sqrt{\ell_i}$, $i = 1, 2$.

The low-frequency behaviour of $K(\omega)$ is determined by the asymptotic behaviour of $K(\omega, \ell)$. Defining the asymptotic function $K_a(\omega, \ell)$ according to the conservation law of Eq. (2.90) as

$$K_a(\omega, \ell) \equiv \frac{1}{\pi}\mathrm{Im}\frac{(h(\ell) - S_1(\omega^2 - i0, \ell))^2}{m(\omega^2 - \omega(\ell)^2) - R(\omega^2 - i0, \ell)} \quad , \tag{2.110}$$

we readily identify

$$K_a(\omega, \ell_1) = K(\omega, \ell_2 = \infty) - K(\omega, \ell_1) \propto \omega^s \quad , \text{as} \quad \omega \to 0 \quad . \tag{2.111}$$

For $s \to 0$ and $\omega \to 0$, we have $K_a(\omega, \ell)/\omega^s \to d^2/2$. For $s = 2$ and $\omega \to 0$, we have $K_a(\omega, \ell)/\omega^2 \to 0$.

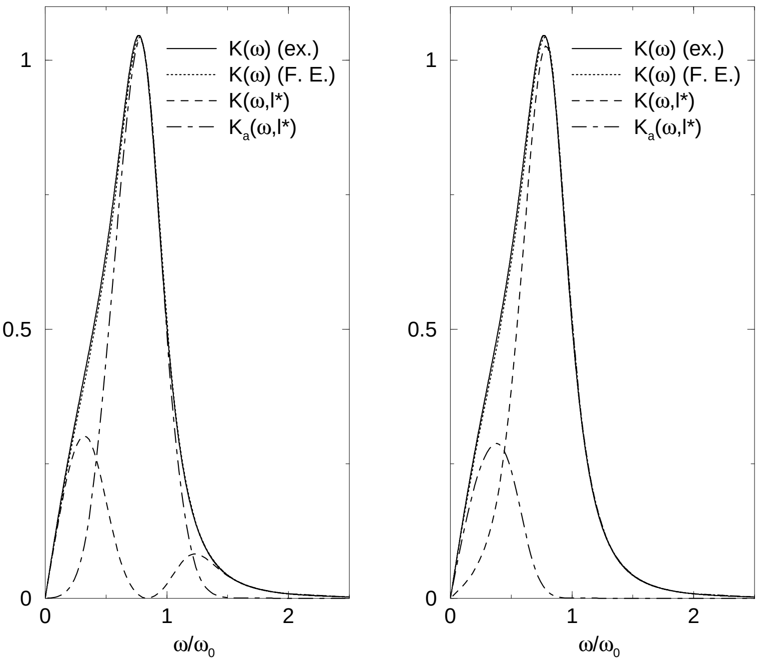

Figure 2.1.: The Spectral Function $K(\omega)$ calculated via Flow Equations with $f(\omega,\ell) = -(\omega-\omega(\ell))/(\omega+\omega(\ell))$ (left hand side) and with $f(\omega,\ell) = -1$ (right hand side), taken at $\ell^* = 10/\omega_0^2$ for $J(\omega) = 4\gamma^2\omega\alpha/(\gamma^2+\omega^2)$ with $\omega_0 \equiv \omega(\ell=0)$, $\alpha = 0.1$ and $\gamma/\omega_0 = 1$ (dotted line). The solid line resembles the analytic solution of Eq. (2.94).

2.3.3. Numerical Results

Exactly solvable models serve as an excellent check for integration routines, which are going to be employed in the later chapters. Throughout this work we will use the C-Routine CVODE, designed to solve stiff differential equations based on Adams- and Backwards-Differentiation.

We first want to calculate the spectral function $K(\omega)$, defined in Eq. (2.92). Given the Lorentzian spectral function as initial coupling function of Eq. (2.93), we will calculate $K(\omega)$ within the Flow Equation approach for two different choices of $f(\omega,\ell)$. To do so we will employ the conservation law of Eq. (2.90), i.e. $K(\omega) = K(\omega,\ell)+K_a(\omega,\ell)$. This allows us to halt the integration routine after a finite ℓ^* and thus circumvent questions about the asymptotic properties of the numerical routines. Nevertheless the final result must be independent of ℓ^*. which is indeed the case.

In Figure 2.1 the two different versions of our Flow Equations are compared. The parameters for the initial coupling $J(\omega)$ are chosen to be $\alpha = 0.1$ and $\gamma/\omega_0 = 1.0$ according to Ref. [Keh97]. The small deviations between the exact solution given in

[4] The minus sign in the equation for the constants a and b would yield $c = d$ which we want to rule out even for $s = 1$.

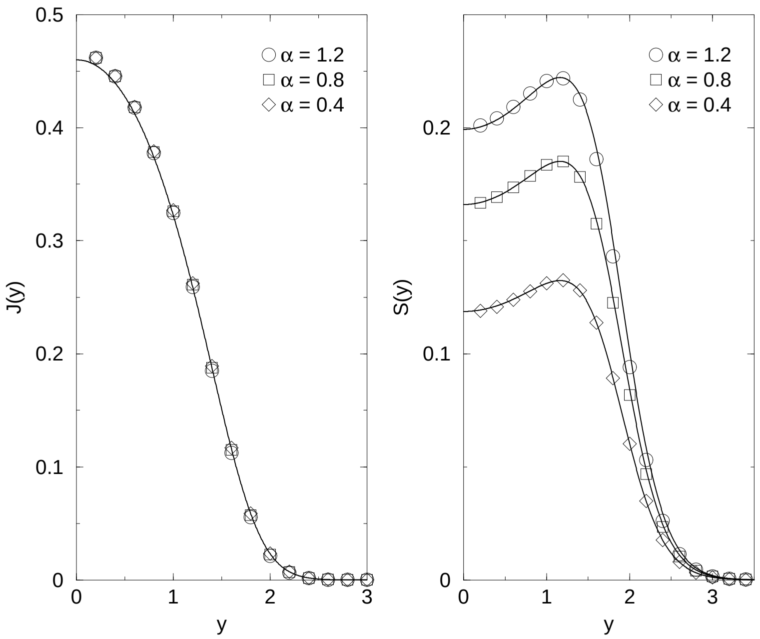

Figure 2.2.: The asymptotic functions $J(y)$ and $S(y)$ at $\ell^* = 100/v_0$ for Ohmic coupling $J(\omega) = 2\alpha\omega\Theta(\omega_c - \omega)$ with $\omega_c^2/v_0 = 100$ and $v_0 \equiv \sigma v(\ell = 0)/m$ for different coupling strengths α. The solid lines resemble the "analytic" solution.

Eq. (2.94) and the solution obtained by Flow Equations are due to the finite cutoff ω_c which had to be introduced in the numerical solution. Our choice $\omega_c/\omega_0 = 50$ does not resemble any limit of numerical capacity and can be easily extended.

The composed spectral function $K(\omega) = K(\omega, \ell) + K_a(\omega, \ell)$ turns out to be indeed independent of the two choices of $f(\omega, \ell)$. Nevertheless they are composed by different functions $K(\omega, \ell)$ and $K_a(\omega, \ell)$. For $f(\omega, \ell) = -(\omega - \omega(\ell))/(\omega + \omega(\ell))$ the weight of the intermediate time scale is mostly contained in $K_a(\omega, \ell)$, whereas for $f(\omega, \ell) = -1$ the asymptotic function $K_a(\omega, \ell)$ determines the long-time behaviour.

After we have shown that the results for $K(\omega)$ are independent of $f(\omega, \ell)$ we want to investigate the asymptotic properties of the Flow Equations for $f(\omega, \ell) = -1$. The differential equations (2.101) and (2.107) can be solved numerically via self-consistent iteration. Comparing these "analytic" results with the numerical results obtained through integrating the Flow Equations serves as a proof that we have found the right universal asymptotic behaviour.

The asymptotic functions given in the last subsection still depend on the parameter s, which also governs the behaviour of the asymptotic spectral function $K_a(\omega)$ for small ω as can be seen from Eq. (2.109). The behaviour of $K(\omega)$ for small ω is known from the analytic solution of the model and corresponds to that of the initial

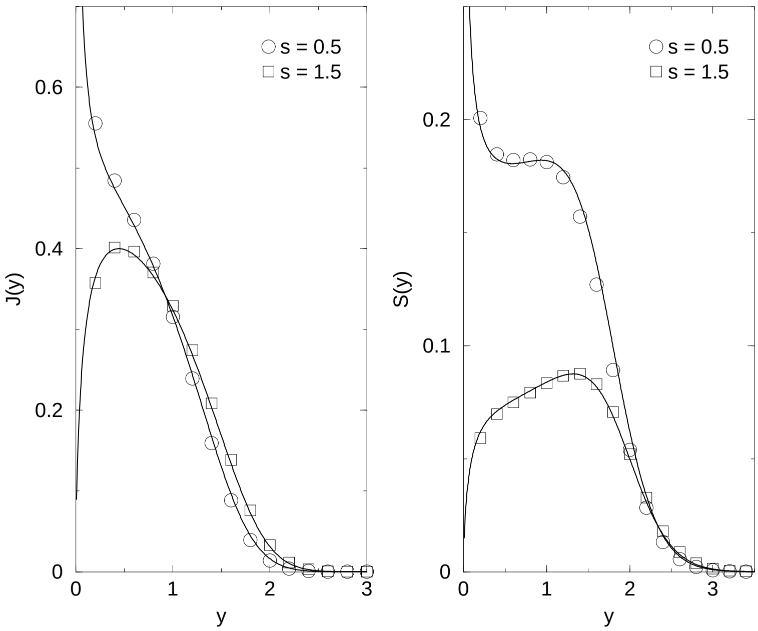

Figure 2.3.: The asymptotic functions $J(y)$ and $S(y)$ at $\ell^* = 100/v_0$ for $J(\omega) = 2\alpha K^{1-s}\omega^s\Theta(\omega_c - \omega)$ with $\alpha = 0.4$, $K = 1$, $\omega_c^2/v_0 = 100$ and $v_0 \equiv \sigma v(\ell = 0)/m$ for different coupling types s. The solid lines resemble the "analytic" solution.

spectral function $J(\omega)$. Since many physical effects, like localization in the Spin-Boson Model, only depend on the low-energy modes of the bath, $J(\omega)$ is often parameterized by just three parameters: the bath or coupling type s, the coupling strength α and K respectively[5] and the cutoff frequency ω_c. One thus often starts with the initial spectral function $J(\omega) \propto 2\alpha K^{1-s}\omega^s f(\omega/\omega_c)$, where $f(x)$ denotes a particular cutoff function with $f(x) \ll 1$ for $x \gg 1$.

As could already be seen from the discussion of the asymptotic behaviour of the Flow Equations, $s = 1$ represents a marginal point. One therefore distinguishes three characteristic coupling types:

- $s > 1$: super-Ohmic coupling
- $s = 1$: Ohmic coupling
- $s < 1$: sub-Ohmic coupling

Our numerical results show that the parameter s, that appears in the asymptotic functions has to be chosen according to the parameter s, that appears in the initial

[5] K gives an additional energy scale for $s \neq 1$ but can also be viewed as a coupling strength. In the following we will set $K = 1$ and define the coupling strength over α.

spectral function. This is reasonable since there is no renormalization of the bath parameters so that the type of the coupling should remain the same.

The results for Ohmic coupling are shown in Figure 2.2 where we plotted the asymptotic curves $J(y)$ and $S(y)$ obtained through direct integration and through self-consistent iteration for different coupling strengths α. Indeed, $J(y)$ is universal for all coupling strengths, the functions $S(y)$ only differ by the constant S_0. This also holds for $s \neq 1$, which is not shown here.

In Figure 2.3 we plotted the asymptotic curves $J(y)$ and $S(y)$ for fixed coupling strength $\alpha = 0.4$, but for two different parameters s. In the super-Ohmic case $s = 1.5$ $J(y)$ and $S(y)$ show a suppression whereas in the sub-Ohmic case $s = 0.5$ $J(y)$ and $S(y)$ diverge as $y \to 0$.

3. Rabi Model

When Flow Equations are applied to non-trivial models, approximations become necessary. In this instance one needs to cut the hierarchy of newly generated interaction terms and then neglect operators, which are assumed to be *irrelevant*. Yet there is no satisfactory definition for *irrelevant operators* within the Flow Equation approach. Especially in order to close the Flow Equations for observables, crude approximations are often unavoidable since emphasis is normally placed on the diagonalization of the Hamiltonian.

So far approximations were justified when certain sum rules, mostly steming from the invariance of commutation relations during the unitary flow, hold exactly or at least asymptotically [Rag99]. In addition, exact relations between static and dynamic properties (as the generalized Shiba relation in the case of the Spin-Boson Model) can serve as justification for prior approximations [Keh97]. A general consistency check lies in the investigation of the flow of the neglected operators.

This chapter addresses the question more specifically. Namely, we will consider an explicit model which is similar to the dissipative models to be investigated in the next chapters - but still exactly solvable via numerical diagonalization. Like this we can test different approximation schemes and compare the results with the numerically exact solution.

This strategy was first pursued by Richter in his diploma work [Ric97]. We will extend his work to Hamiltonians where the reflection symmetry is broken. This is important if one wants to understand the mechanism of phase transition as being observed in the Spin-Boson Model.

We will present a particular truncation scheme which remains invariant with respect to the particular choice of initial Hamiltonians, provided that they only vary by a unitary transformation. Furthermore, a general truncation scheme is proposed which generally yields the best result. As a criterion for the quality of the Flow Equations, we look at the ground state energy as function of the bias ϵ as an example for the flow of a parameter of the Hamiltonian.

Further, we will give a thorough discussion about the flow of the observables. As reference we will not only rely on sum rules which stem from the commutation relations - but also compare the Flow Equation result with the exact solution. For this, an expansion of the operator into a basis of normal ordered bosonic operators is given.

3.1. Flow of the Hamiltonian

The Spin-Boson Hamiltonian with only one mode, which we will call the Rabi Model in order to distinguish it from the Spin-Boson Model with an arbitrary number of modes discussed in the next chapter, shall be given by

$$H = -\frac{\Delta_0}{2}\sigma_x + \frac{\epsilon_0}{2}\sigma_z + \omega_0 b^\dagger b + \sigma_z\frac{\lambda_0}{2}(b + b^\dagger) + E_0 \quad . \tag{3.1}$$

The operator $b^{(\dagger)}$ resembles the bosonic degree of freedom and σ_i with $i = x, y, z$ denote the Pauli spin matrices. They obey the canonical commutation relation $[b, b^\dagger] = 1$ and the spin-1/2 algebra $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$. Below we will also use the following representation of the Pauli spin matrices: $\sigma_x \equiv c_1^\dagger c_0 + c_0^\dagger c_1$, $i\sigma_y \equiv c_0^\dagger c_1 - c_1^\dagger c_0$ and $\sigma_z \equiv c_0^\dagger c_0 - c_1^\dagger c_1$. The $c_i^{(\dagger)}$ with $i = 0, 1$ obey the canonical anti-commutation relations $\{c_i^\dagger, c_j\} = \delta_{i,j}$. Further we have $1 = c_0^\dagger c_0 + c_1^\dagger c_1$, in order to restrict the fermionic Hilbert space.

The Flow Equations are generated by the anti-hermitian operator η which is canonically given by $\eta = [H_0, H]$, where H_0 defines the diagonal Hamiltonian. The objective is to decouple the fermionic system from the bosonic system, i.e. $\lambda_0(\ell) \to 0$ for $\ell \to \infty$.

Obviously different choices for H_0 can lead to different Flow Equations. In the first subsection we will therefore discuss three different versions of the free one-particle Hamiltonian and their implications on the canonical generator and thus on the Flow Equations. We will also include Flow Equations which leave the initial Hamiltonian form-invariant.

In the second subsection we want to determine how the flow changes if parity is not conserved even if no bias ϵ_0 is applied. For that we shift the bosonic mode $b \to b - \frac{\lambda_0}{2\omega_0}$ which yields the with respect to (3.1) unitarily equivalent Hamiltonian

$$\begin{aligned} H &= -\frac{\Delta_0}{2}\sigma_x + \frac{\epsilon_0}{2}\sigma_z + \omega_0(b^\dagger - c_1^\dagger c_1\frac{\lambda_0}{\omega_0})(b - c_1^\dagger c_1\frac{\lambda_0}{\omega_0}) - \frac{\lambda_0^2}{4\omega_0} + E_0 \\ &= -\frac{\Delta_0}{2}\sigma_x + c_1^\dagger c_1\Lambda_0 + \omega_0 b^\dagger b - c_1^\dagger c_1\lambda_0(b + b^\dagger) + E_0' \quad . \end{aligned} \tag{3.2}$$

In Eq. (3.2) we defined $\Lambda_0 \equiv \lambda_0^2/\omega_0 - \epsilon_0$ and $E_0' \equiv E_0 + \frac{\epsilon_0}{2} - \frac{\lambda_0^2}{4\omega_0}$. Again we will discuss three different versions of the free one-particle Hamiltonian, this time with the bosonic mode shifted.

3.1.1. Flow Equations for Un-shifted Mode

The Rabi Model is not exactly solvable. This is expressed by the fact that the Flow Equations generate an infinite hierarchy of new interaction terms which cannot be summed to yield a closed form, as it was e.g. the case of the operator flow of the Independent Boson Model. We therefore need to truncate the Flow Equations. And in the following subsection we will consider the flow of all interaction terms which are linear in the bosonic operator $b^{(\dagger)}$. The truncated Hamiltonian shall thus be given by

$$\begin{aligned} H = &-\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b + E \\ &+ \frac{\lambda^e}{2}(b+b^\dagger) + \sigma_x\frac{\lambda^x}{2}(b+b^\dagger) + i\sigma_y\frac{\lambda^y}{2}(b-b^\dagger) + \sigma_z\frac{\lambda^z}{2}(b+b^\dagger) \quad , \end{aligned} \tag{3.3}$$

where the initial conditions will be specified later.

The flow shall be governed by the generator

$$\begin{aligned} \eta &= i\sigma_y\eta^{0,y} + \eta^e(b-b^\dagger) + \sigma_x\eta^x(b-b^\dagger) + i\sigma_y\eta^y(b+b^\dagger) + \sigma_z\eta^z(b-b^\dagger) \\ &\equiv \hat{\eta}^{0,y} + \hat{\eta}^e + \hat{\eta}^x + \hat{\eta}^y + \hat{\eta}^z \quad , \end{aligned} \tag{3.4}$$

where the parameters $\eta^{0,y}$, η^e, η^x, η^y, and η^z will be specified later.

Eq. (3.4) represents the most general anti-hermitian operator which includes all possible operators acting on the underlying Hilbert space up to linear bosonic operators. The commutator $[\eta, H]$ yields the following contributions:

$$[\hat{\eta}^{0,y}, H] = -\sigma_z\Delta\eta^{0,y} - \sigma_x\epsilon\eta^{0,y} + \sigma_z\eta^{0,y}\lambda^x(b+b^\dagger) - \sigma_x\eta^{0,y}\lambda^z(b+b^\dagger) \tag{3.5}$$

$$[\hat{\eta}^e, H] = \eta^e\omega_0(b+b^\dagger) + \eta^e\lambda^e + \sigma_x\eta^e\lambda^x + \sigma_z\eta^e\lambda^z \tag{3.6}$$

$$\begin{aligned} [\hat{\eta}^x, H] = &-i\sigma_y\epsilon\eta^x(b-b^\dagger) + \sigma_x\eta^x\omega_0(b+b^\dagger) \\ &+ \sigma_x\eta^x\lambda^e + \eta^x\lambda^x - \sigma_z\eta^x\lambda^y(b-b^\dagger)^2 - i\sigma_y\eta^x\frac{\lambda^z}{2}\{(b-b^\dagger),(b+b^\dagger)\} \end{aligned} \tag{3.7}$$

$$\begin{aligned} [\hat{\eta}^y, H] = &-\sigma_z\Delta\eta^y(b+b^\dagger) - \sigma_x\epsilon\eta^y(b+b^\dagger) + i\sigma_y\eta^y\omega_0(b-b^\dagger) \\ &+ \sigma_z\eta^y\lambda^x(b+b^\dagger)^2 + \eta^y\lambda^y - \sigma_x\eta^y\lambda^z(b+b^\dagger)^2 \end{aligned} \tag{3.8}$$

$$\begin{aligned} [\hat{\eta}^z, H] = &-i\sigma_y\Delta\eta^z(b-b^\dagger) + \sigma_z\eta^z\omega_0(b+b^\dagger) + \sigma_z\eta^z\lambda^e \\ &+ i\sigma_y\eta^z\frac{\lambda^x}{2}\{(b-b^\dagger),(b+b^\dagger)\} + \sigma_x\eta^z\lambda^y(b-b^\dagger)^2 + \eta^z\lambda^z \end{aligned} \tag{3.9}$$

To close the Flow Equations we will neglect the normal ordered operators

$$\mathcal{O}_1 = -\sigma_x\eta^y\lambda^z : (b+b^\dagger)^2 : \quad , \quad \mathcal{O}_2 = \sigma_z\eta^y\lambda^x : (b+b^\dagger)^2 : \quad , \tag{3.10}$$

$$\mathcal{O}_3 = \sigma_x\eta^z\lambda^y : (b-b^\dagger)^2 : \quad , \quad \mathcal{O}_4 = -\sigma_z\eta^x\lambda^y : (b-b^\dagger)^2 : \quad , \tag{3.11}$$

$$\mathcal{O}_5 = i\sigma_y(\eta^z\frac{\lambda^x}{2} - \eta^x\frac{\lambda^z}{2}) : \{(b-b^\dagger),(b+b^\dagger)\} : \quad . \tag{3.12}$$

Normal ordering is defined as $:(b+b^\dagger)^2 :\equiv (b+b^\dagger)^2 - \langle(b+b^\dagger)^2\rangle$, with $\langle(b+b^\dagger)^2\rangle = 1+2n$ and $n = (e^{\beta\omega_0}-1)^{-1}$ being the Bose factor. The above truncation scheme has the effect that the bosonic energy ω_0 is not being renormalized during the flow. This might seem to be a short-come of the Flow Equations, but since in this work we are focused on dissipative systems where the bath parameters are indeed left un-renormalized, we would like to keep this scheme in view of the later Flow Equations.

With $\partial_\ell H = [\eta, H]$ we obtain the following Flow Equations:

$$\partial_\ell \Delta = 2\epsilon\eta^{0,y} - 2\eta^e\lambda^x - 2\eta^x\lambda^e + 2(\eta^z\lambda^y + \eta^y\lambda^z)(1+2n) \tag{3.13}$$
$$\partial_\ell \epsilon = -2\Delta\eta^{0,y} + 2\eta^z\lambda^e + 2(\eta^y\lambda^x + \eta^x\lambda^y)(1+2n) + 2\eta^e\lambda^z \tag{3.14}$$
$$\partial_\ell \lambda^x = -2\epsilon\eta^y + 2\eta^x\omega_0 - 2\eta^{0,y}\lambda^z \quad , \quad \partial_\ell\lambda^y = -2\Delta\eta^z - 2\epsilon\eta^x + 2\eta^y\omega_0 \tag{3.15}$$
$$\partial_\ell \lambda^z = -2\Delta\eta^y + 2\eta^z\omega_0 + 2\eta^{0,y}\lambda^x \quad , \quad \partial_\ell E = \eta^e\lambda^e + \eta^x\lambda^x + \eta^y\lambda^y + \eta^z\lambda^z \tag{3.16}$$

Including $\partial_\ell\lambda^e = 2\eta^e\omega_0$, this is the most general form of the Flow Equations following the above truncation scheme.[1] With $\lambda^e = \eta^e = 0$, an obvious invariant is given by $\text{Inv} = \Delta^2 + \epsilon^2 + \lambda^{x2} + \lambda^{y2} + \lambda^{z2} - 4E\omega_0$. To investigate the Flow Equations further, one has to specify the constants and initial conditions. To do so we will choose different diagonal Hamiltonians H_0 and we will compare them by means of the ground-state energy of the system.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \omega_0 b^\dagger b}$

One obvious choice is to set the diagonal Hamiltonian to be $H_0 = -\frac{\Delta}{2}\sigma_x + \omega_0 b^\dagger b$. Considering the Hamiltonian (3.3), the initial Rabi Hamiltonian (3.1) is given by setting $\Delta = \Delta_0$, $\epsilon = \epsilon_0$, $E = E_0$, $\lambda^z = \lambda_0$ and $\lambda^e = \lambda^x = \lambda^y = 0$ for $\ell = 0$. The canonical generator $\eta = [H_0, H]$ follows from the generator given in Eq. (3.4) by setting $\eta^{0,y} = \Delta\epsilon/2$, $\eta^e = -\omega_0\lambda^e/2$, $\eta^x = -\omega_0\lambda^x/2$, $\eta^y = (\Delta\lambda^z - \omega_0\lambda^y)/2$ and $\eta^z = (-\omega_0\lambda^z + \Delta\lambda^y)/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1a.

- $\boldsymbol{H_0 = \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b}$

Another choice for the diagonal Hamiltonian is given by $H_0 = \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b$. Considering the Hamiltonian (3.3), the initial Rabi Hamiltonian (3.1) is given by setting $\Delta = \Delta_0$, $\epsilon = \epsilon_0$, $E = E_0$, $\lambda^z = \lambda_0$ and $\lambda^e = \lambda^x = \lambda^z = 0$ for $\ell = 0$. The canonical generator $\eta = [H_0, H]$ follows from the generator given in Eq. (3.4) by setting $\eta^{0,y} = -\Delta\epsilon/2$, $\eta^e = -\omega_0\lambda^e/2$, $\eta^x = (-\omega_0\lambda^x + \epsilon\lambda^y)/2$, $\eta^y = (\epsilon\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = -\omega_0\lambda^z/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1b.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b}$

Combining the previous choices we arrive at the diagonal Hamiltonian $H_0 = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b$. Since the Pauli spin matrices do not commute, we will first diagonalize the one-particle Hamiltonian $H_0^p = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z \to \frac{R}{2}\sigma_z$ with $R = \sqrt{\Delta^2 + \epsilon^2}$ the Rabi frequency.[2] Considering the Hamiltonian (3.3), and replacing ϵ by R since the operator σ_z does not resemble an applied bias anymore, the initial Rabi Hamiltonian (3.1) is

[1] In the following discussion we will have $\lambda^e = \eta^e = 0$ for all ℓ.

[2] To recall the algebra of the two-level system Appendix B was added.

then obtained by setting $\Delta = 0$, $R = R_0$, $E = E_0$, $\lambda^e = 0$, $\lambda^x \equiv \lambda_0\Delta_0/R_0$, $\lambda^y = 0$ and $\lambda^z \equiv \lambda_0\epsilon_0/R_0$ with $R_0 = \sqrt{\Delta_0^2 + \epsilon_0^2}$. The canonical generator $\eta = [H_0, H]$ is obtained from the generator given in Eq. (3.4) by setting $\eta^{0,y} = -\Delta R/2$, $\eta^e = -\omega_0\lambda^e/2$, $\eta^x = (-\omega_0\lambda^x + R\lambda^y)/2$, $\eta^y = (R\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = -\omega_0\lambda^z/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1c.

- **Form-Invariant Flow**

If we want the initial Hamiltonian (3.1) to remain form-invariant, the constants of the generator have to satisfy the following relations:

$$\Delta\eta^z + \epsilon\eta^x - \eta^y\omega_0 = 0 \quad , \quad \epsilon\eta^y - \eta^x\omega_0 + \eta^{0,y}\lambda^z = 0 \tag{3.17}$$

With these relations, the constants are defined up to a constant f. If one chooses $\eta^z = -\omega_0\lambda^z f/2$ one finds $\eta^{0,y} = \epsilon\Delta f/2$, $\eta^e = 0$, $\eta^x = 0$ and $\eta^y = -\Delta\lambda^z f/2$. With this choice, all neglected operators except of $\mathcal{O}_1$ vanish. One obtains the following coupled differential equations:

$$\begin{aligned} \partial_\ell\Delta &= -\Delta\lambda^{z2} f(1+2n) + \Delta\epsilon^2 f \quad , \quad \partial_\ell\epsilon = -\epsilon\Delta^2 f \\ \partial_\ell\lambda^z &= \lambda^z(\Delta^2 - \omega_0^2) f \quad , \quad \partial_\ell E = -\omega_0\lambda^{z2} f/2 \end{aligned} \tag{3.18}$$

In the following we set $f = 1$ and refer to this set of Flow Equation as Version 1d.

We want to consider the form-invariant flow after having transformed the one-particle Hamiltonian as described in Version 1c. If we want to avoid the generation of Δ and λ^y one needs the conditions $\Delta\eta^z + R\eta^x - \eta^y\omega_0 = 0$ and $R\eta^{0,y}(1+2n) + \eta^y\lambda^z = 0$. Again the parameters of the generator are only defined up to a constant. Choosing $\eta^e = 0$, $\eta^x = -\omega_0\lambda^x f/2$, $\eta^z = -\omega_0\lambda^z f/2$ renders $\mathcal{O}_5$ zero and yields $\eta^{0,y} = \lambda^x\lambda^z f(1+2n)/2$ and $\eta^y = -R\lambda^x f/2$. Thus all neglected operators but $\mathcal{O}_1$ and $\mathcal{O}_2$ are zero. We obtain the following Flow Equations:

$$\begin{aligned} &\partial_\ell R = -R\lambda^{x2} f(1+2n) \quad , \quad \partial_\ell E = -\omega_0(\lambda^{x2} + \lambda^{z2}) f/2 \\ &\partial_\ell\lambda^x = -\omega_0^2\lambda^x f + R^2\lambda^x f - \lambda^{z2}\lambda^x f(1+2n) \quad , \quad \partial_\ell\lambda^z = -\omega_0^2\lambda^z f + \lambda^{x2}\lambda^z f(1+2n) \end{aligned} \tag{3.19}$$

The set of equations in (3.19) is equivalent to the set of equations in (3.18). This can be seen by introducing "new" variables $\Delta' = \lambda^x R/\lambda'$, $\epsilon' = \lambda^z R/\lambda'$ and $\lambda'^2 = \lambda^{x2} + \lambda^{z2}$ and setting up their differential equations, which coincide with (3.18). This is a remarkable result. It demonstrates that keeping the Hamiltonian form-invariant during the flow preserves the unitary equivalence with respect to the two-dimensional Hilbert space of the spin degree of freedom of the initial Hamiltonians.

3.1.2. Flow Equations for Shifted Mode

If no approximations are made the canonical Flow Equations do not depend on the representation of the initial Hamiltonian if only the diagonal Hamiltonian H_0 remains equal. We have seen that truncated Flow Equations can be equivalent even though the initial Hamiltonians differ by a unitary transformation in the two-dimensional fermionic Hilbert space. We want to investigate this further by performing a unitary transformation on the bosonic Hilbert space. By shifting the bosonic modes we can also address the aspect of symmetry and Flow Equations because the reflection symmetry is broken even for $\epsilon_0 = 0$. As a consequence we will see that the flow of the Hamiltonian will cover the whole truncated operator space and not leave $\lambda^e = 0$, as in the previous subsection.

We will thus set up Flow Equations for the initial Hamiltonian given in Eq. (3.2). The truncated Hamiltonian shall then be given by

$$\begin{aligned} H &= -\frac{\Delta}{2}\sigma_x + \Lambda c_1^\dagger c_1 + \omega_0 b^\dagger b + E \\ &+ \frac{\lambda^e}{2}(b+b^\dagger) + \sigma_x\frac{\lambda^x}{2}(b+b^\dagger) + i\sigma_y\frac{\lambda^y}{2}(b-b^\dagger) - c_1^\dagger c_1\lambda^z(b+b^\dagger) \quad . \end{aligned} \tag{3.20}$$

The flow shall again be governed by the generator

$$\begin{aligned} \eta &= i\sigma_y\eta^{0,y} + \eta^e(b-b^\dagger) + \sigma_x\eta^x(b-b^\dagger) + i\sigma_y\eta^y(b+b^\dagger) + \sigma_z\eta^z(b-b^\dagger) \\ &\equiv \hat\eta^{0,y} + \hat\eta^e + \hat\eta^x + \hat\eta^y + \hat\eta^z \quad . \end{aligned} \tag{3.21}$$

The commutator $[\eta, H]$ yields the following contributions:

$$[\hat\eta^{0,y}, H] = -\sigma_z\Delta\eta^{0,y} + \sigma_x\Lambda\eta^{0,y} + \sigma_z\eta^{0,y}\lambda^x(b+b^\dagger) - \sigma_x\eta^{0,y}\lambda^z(b+b^\dagger) \tag{3.22}$$

$$[\hat\eta^e, H] = \eta^e\omega_0(b+b^\dagger) + \eta^e\lambda^e + \sigma_x\eta^e\lambda^x - 2c_1^\dagger c_1\eta^e\lambda^z \tag{3.23}$$

$$\begin{aligned} [\hat\eta^x, H] &= i\sigma_y\Lambda\eta^x(b-b^\dagger) + \sigma_x\eta^x\omega_0(b+b^\dagger) + \sigma_x\eta^x\lambda^e + \eta^x\lambda^x \\ &- \sigma_z\eta^x\lambda^y(b-b^\dagger)^2 - i\sigma_y\eta^x\frac{\lambda^z}{2}\{(b-b^\dagger),(b+b^\dagger)\} - \sigma_x\eta^x\lambda^z \end{aligned} \tag{3.24}$$

$$\begin{aligned} [\hat\eta^y, H] &= -\Delta\sigma_z\eta^y(b+b^\dagger) + \sigma_x\Lambda\eta^y(b+b^\dagger) + i\sigma_y\eta^y\omega_0(b-b^\dagger) \\ &+ \sigma_z\eta^y\lambda^x(b+b^\dagger)^2 + \eta^y\lambda^y - \sigma_x\eta^y\lambda^z(b+b^\dagger)^2 \end{aligned} \tag{3.25}$$

$$\begin{aligned} [\hat\eta^z, H] &= -i\sigma_y\Delta\eta^z(b-b^\dagger) + \sigma_z\eta^z\omega_0(b+b^\dagger) + \sigma_z\eta^z\lambda^e + \sigma_x\eta^z\lambda^y(b-b^\dagger)^2 \\ &+ i\sigma_y\eta^z\frac{\lambda^x}{2}\{(b-b^\dagger),(b+b^\dagger)\} + 2c_1^\dagger c_1\eta^z\lambda^z \end{aligned} \tag{3.26}$$

In order to close the Flow Equations we will again neglect normal ordered bosonic bilinears. But since we have shifted the bosonic Hamiltonian this will be done with respect to the free Hamiltonian of the *shifted* bosonic modes. This Hamiltonian reads

$$H_B = \omega_0(b^\dagger - \langle c_1^\dagger c_1\rangle\frac{\lambda^z}{\omega_0})(b - \langle c_1^\dagger c_1\rangle\frac{\lambda^z}{\omega_0}) \quad . \tag{3.27}$$

We thus neglect the normal ordered operators

$$\mathcal{O}_1 = -\sigma_x\eta^y\lambda^z :(\bar b + \bar b^\dagger)^2: \quad , \quad \mathcal{O}_2 = \sigma_z\eta^y\lambda^x :(\bar b + \bar b^\dagger)^2: \quad , \tag{3.28}$$

$$\mathcal{O}_3 = \sigma_x\eta^z\lambda^y :(\bar b - \bar b^\dagger)^2: \quad , \quad \mathcal{O}_4 = -\sigma_z\eta^x\lambda^y :(\bar b - \bar b^\dagger)^2: \quad , \tag{3.29}$$

$$\mathcal{O}_5 = i\sigma_y(\eta^z\frac{\lambda^x}{2} - \eta^x\frac{\lambda^z}{2}) :\{(\bar b - \bar b^\dagger),(\bar b + \bar b^\dagger)\}: \quad , \tag{3.30}$$

with $\bar{b} \equiv b - \langle c_1^\dagger c_1 \rangle \frac{\lambda^z}{\omega_0}$. With $\partial_\ell H = [\eta, H]$ we obtain the following Flow Equations:

$$\partial_\ell \Delta = 2(-\Lambda\eta^{0,y} - \eta^x\lambda^e - \eta^e\lambda^x + (\eta^z\lambda^y + \eta^y\lambda^z)1_n + \eta^x\lambda^z - \eta^y\lambda^z\delta^2) \tag{3.31}$$
$$\partial_\ell \Lambda = 2(\Delta\eta^{0,y} - \eta^z\lambda^e - (\eta^y\lambda^x + \eta^x\lambda^y)1_n + \eta^z\lambda^z - \eta^e\lambda^z + \eta^y\lambda^x\delta^2) \tag{3.32}$$
$$\partial_\ell \lambda^e = 2(-\eta^y\Delta + \eta^z\omega_0 + \eta^e\omega_0 + \eta^{0,y}\lambda^x - 2\eta^y\lambda^x\delta) \tag{3.33}$$
$$\partial_\ell \lambda^x = 2(\Lambda\eta^y + \eta^x\omega_0 - \eta^{0,y}\lambda^z + 2\eta^y\lambda^z\delta) \tag{3.34}$$
$$\partial_\ell \lambda^y = 2(-\Delta\eta^z + \Lambda\eta^x + \eta^y\omega_0 - \eta^z\lambda^x\delta + \eta^x\lambda^z\delta) \tag{3.35}$$
$$\partial_\ell \lambda^z = 2(-\Delta\eta^y + \eta^z\omega_0 + \eta^{0,y}\lambda^x - 2\eta^y\lambda^x\delta) \tag{3.36}$$
$$\partial_\ell E = -\Delta\eta^{0,y} + \eta^e\lambda^e + \eta^z\lambda^e + \eta^y\lambda^x 1_n - \eta^y\lambda^x\delta^2 + \eta^x\lambda^x + \eta^y\lambda^y + \eta^x\lambda^y 1_n \quad , \tag{3.37}$$

where we defined $\delta \equiv -2\langle c_1^\dagger c_1\rangle \frac{\lambda^z}{\omega_0}$ and $1_n \equiv 1 + 2n$ with n denoting the Bose factor.

In order to discuss the Flow Equations in detail, we will now specify the constants of the generator. Again we will choose three different diagonal Hamiltonians and then determine the constants of the canonical generator. We will further address the question of equivalence of the two scheme, shifted and un-shifted bosonic modes, on grounds of the form-invariant flow of the Hamiltonian.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \omega_0 b^\dagger b}$

An obvious choice for the diagonal Hamiltonian is given by $H_0 = -\frac{\Delta}{2}\sigma_x + \omega_0 b^\dagger b$. Considering the Hamiltonian (3.20), the initial Rabi Hamiltonian (3.2) is given by setting $\Delta = \Delta_0$, $\Lambda = \Lambda_0$, $E = E_0'$, $\lambda^z = \lambda_0$ and $\lambda^e = \lambda^x = \lambda^z = 0$ for $\ell = 0$. The canonical generator $\eta = [H_0, H]$ is obtained from the generator given in Eq. (3.21) by setting $\eta^{0,y} = -\Delta\Lambda/2$, $\eta^e = -\omega_0(\lambda^e - \lambda^z)/2$, $\eta^x = -\omega_0\lambda^x/2$, $\eta^y = (\Delta\lambda^z - \omega_0\lambda^y)/2$ and $\eta^z = (-\omega_0\lambda^z + \Delta\lambda^y)/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 2a.

- $\boldsymbol{H_0 = \Lambda c_1^\dagger c_1 + \omega_0 b^\dagger b}$

Another choice for the diagonal Hamiltonian is given by $H_0 = \Lambda c_1^\dagger c_1 + \omega_0 b^\dagger b$. Considering the Hamiltonian (3.20), the initial Rabi Hamiltonian (3.2) is given by setting $\Delta = \Delta_0$, $\Lambda = \Lambda_0$, $E = E_0'$, $\lambda^z = \lambda_0$ and $\lambda^x = \lambda^y = 0$ for $\ell = 0$. The canonical generator $\eta = [H_0, H]$ is obtained from the generator given in Eq. (3.21) by setting $\eta^{0,y} = \Delta\Lambda/2$, $\eta^e = -\omega_0(\lambda^e - \lambda^z)/2$, $\eta^x = (-\omega_0\lambda^x - \Lambda\lambda^y)/2$, $\eta^y = (-\Lambda\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = -\omega_0\lambda^z/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 2b.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \Lambda c_1^\dagger c_1 + \omega_0 b^\dagger b}$

The largest obvious diagonal Hamiltonian is given by $H_0 = -\frac{\Delta}{2}\sigma_x + \Lambda c_1^\dagger c_1 + \omega_0 b^\dagger b$. Again we will first diagonalize the Hamiltonian $H_0^p = -\frac{\Delta}{2}\sigma_x + \Lambda c_1^\dagger c_1 \to \frac{\Lambda}{2} - \frac{R}{2}\sigma_z$ with $R = \sqrt{\Delta^2 + \Lambda^2}$ denoting the Rabi frequency. The transformation of $c_1^\dagger c_1$ is then given by $c_1^\dagger c_1 \to 1/2 - \Delta/(2R)\sigma_x - \Lambda/(2R)\sigma_z$.[3] The initial Hamiltonian of Eq. (3.20) is thus given by $\Delta = 0$, $\Lambda = R_0$, $\lambda^e = -\lambda_0 + \lambda_0\Lambda_0/R_0$, $\lambda^x = \lambda_0\Delta_0/R_0$, $\lambda^y = 0$, $\lambda^z = \lambda_0\Lambda_0/R_0$ and $E = E_0' + \frac{\Lambda_0}{2} - \frac{R_0}{2}$ with $R_0 = \sqrt{\Delta_0^2 + \Lambda_0^2}$. The canonical generator $\eta = [H_0, H]$ is obtained from the generator given in Eq. (3.21) by setting $\eta^{0,y} = \Delta R/2$, $\eta^e = -\omega_0(\lambda^e - \lambda^z)/2$, $\eta^x = (-\omega_0\lambda^x - R\lambda^y)/2$, $\eta^y = (-R\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = -\omega_0\lambda^z/2$. The Flow Equations (3.31) - (3.37) apply if one replaces $\Lambda \to R$. We will refer to the Flow Equations with this particular choice of the generator as Version 2c.

- **Form-Invariant Flow**

If we want to keep the initial Hamiltonian (3.2) to remain form-invariant during the flow, the constants have to satisfy the following relations ($\widetilde{\Lambda} \equiv \lambda^{z2}/\omega_0$) :

$$\eta^z\Delta - \eta^x\Lambda - \eta^y\omega_0 = 0 \tag{3.38}$$

$$\eta^e\omega_0 + \eta^z\omega_0 - \eta^y\Delta = 0 \tag{3.39}$$

$$\eta^{0,y}\lambda^z - \eta^x\omega_0 - \eta^y\Lambda + 2\eta^y\widetilde{\Lambda}(2\langle c_1^\dagger c_1\rangle) = 0 \tag{3.40}$$

If we choose $\eta^y = -\Delta\lambda^z f/2$ we obtain $\eta^z = -\omega_0\lambda^z f/2$, $\eta^x = 0$, $\eta^{0,y} = -\Delta\Lambda f/2 + \Delta\widetilde{\Lambda} f(2\langle c_1^\dagger c_1\rangle)$ and $\eta^e = \omega_0\lambda^z f/2 - \Delta^2\lambda^z f/(2\omega_0)$ with the constant f to be determined later. With $\epsilon = \widetilde{\Lambda} - \Lambda$, this yields the following Flow Equations ($\langle\sigma_z\rangle = 1 - 2\langle c_1^\dagger c_1\rangle$):

$$\begin{aligned} &\partial_\ell\Delta = -\Delta\lambda^{z2} f 1_n + \Delta f(\epsilon + \widetilde{\Lambda}\langle\sigma_z\rangle)^2 \quad , \quad \partial_\ell\epsilon = -\Delta^2\epsilon f - 2\Delta^2\widetilde{\Lambda}\langle\sigma_z\rangle f \quad , \\ &\partial_\ell\lambda^z = \lambda^z(\Delta^2 - \omega_0^2) f \quad , \quad \partial_\ell E = -\Delta^2\widetilde{\Lambda} f/2 + \partial_\ell\epsilon f/2 \end{aligned} \tag{3.41}$$

Recalling the initial condition of the energy shift $E_0' = E_0 + \epsilon/2 - \widetilde{\Lambda}/4$ defined in Eq. (3.3) we see that the Flow Equations are equivalent to the Flow Equations of Version $1d$ if we set $f = 1$ and $\langle\sigma_z\rangle = 0$.

This is a remarkable result. It shows that if one imposes invariance of the Flow Equations with respect to unitarily equivalent initial Hamiltonians and follows the truncation scheme that leaves the Hamiltonian form-invariant, the Flow Equations are uniquely determined. It also shows that normal ordering with respect to the ℓ-dependent Hamiltonian H_B of Eq. (3.27) leads to reasonable results.

So far we have not specified the expectation value $\langle c_1^\dagger c_1\rangle$ that enters the Flow Equations through normal ordering. It should be chosen such that the Flow Equations are invariant with respect to $\epsilon \to -\epsilon$. For the Flow Equations in (3.41) this is the case if $\langle\sigma_z\rangle \propto \epsilon$.

To investigate this further we go back to the initial Hamiltonian given in the first line of Eq. (3.3). Defining the one-particle Hamiltonian $H^p = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}$, we naturally decouple the system by setting $H \approx H^p + H_B$ with H_B given in Eq. (3.27). The expectation value could now be given by $\langle\sigma_z\rangle = -\epsilon/\sqrt{\Delta_r^2 + \epsilon^2}$, where we already included a

[3] To recall the algebra of the two-level system see Appendix B.

possible renormalization of the tunnel-matrix element, e.g. $\Delta_r \equiv \Delta \exp(-\frac{\lambda^2}{2\omega_0^2})$. This implies that the bosonic shift is given by $\delta = -(1+\epsilon/\sqrt{\Delta_r^2+\epsilon^2})\lambda^z/\omega_0$.

Since new interaction terms are being generated a more consistent decoupling scheme of the Hamiltonian , which follows the same considerations as above, is given by ($\langle i\sigma_y \rangle = 0$):

$$H \approx -\frac{\Delta'}{2}\sigma_x + \Lambda' c_1^\dagger c_1 + E'' + \omega_0 (b^\dagger + \frac{\lambda^e}{2\omega_0} + \langle \sigma_x \rangle \frac{\lambda^x}{2\omega_0} - \langle c_1^\dagger c_1 \rangle \frac{\lambda^z}{\omega_0}) \times (b + \frac{\lambda^e}{2\omega_0} + \langle \sigma_x \rangle \frac{\lambda^x}{2\omega_0} - \langle c_1^\dagger c_1 \rangle \frac{\lambda^z}{\omega_0}) \quad , \tag{3.42}$$

with $\Delta' \equiv \Delta + \frac{\lambda^e\lambda^x}{\omega_0} - \frac{\lambda^x\lambda^z}{\omega_0} - \frac{\lambda^y\lambda^z}{\omega_0}$, $\Lambda' \equiv \Lambda + \frac{\lambda^e\lambda^z}{\omega_0} + \frac{\lambda^x\lambda^y}{\omega_0} - \frac{\lambda^z\lambda^z}{\omega_0}$ and $E'' \equiv E' - \frac{\lambda^e\lambda^e}{4\omega_0} - \frac{\lambda^x\lambda^x}{4\omega_0} - \frac{\lambda^y\lambda^y}{4\omega_0}$. Now the bosonic shift δ is given by

$$\delta \equiv \frac{\lambda^e}{\omega_0} + \langle \sigma_x \rangle \frac{\lambda^x}{\omega_0} - 2\langle c_1^\dagger c_1 \rangle \frac{\lambda^z}{\omega_0} \quad , \tag{3.43}$$

with $\langle \sigma_x \rangle = \Delta'/\sqrt{\Delta'^2 + \Lambda'^2}$ and $\langle \sigma_z \rangle = \Lambda'/\sqrt{\Delta'^2 + \Lambda'^2}$.

3.1.3. Numerical Results

We want to analyze the quality of the above Flow Equations by means of the ground-state energy E_g of the system as a function of the external bias ϵ_0. These results are compared with the numerically exact solution obtained via numerical diagonalization. Since the bosonic mode is left un-renormalized the energy scale is given by ω_0. For the coupling constant we choose $\lambda_0 = \omega_0$ which means that we are not in the perturbative regime.

We will first consider the flow of the un-shifted operators discussed in subsection 3.1.1. In Figure 3.1 the ground-state energies E_g^{FE} obtained from the different canonical generators discussed in this subsection are shown. Calculations are done for two different tunnel-matrix elements $\Delta_0 = 0.5\omega_0$ (left hand side) and $\Delta_0 = 1.5\omega_0$ (right hand side), the first below and the second above resonance. Resonance in the uncoupled system is given by $\Delta_0 = \omega_0$. All results are in good agreement with the numerically exact solution. Differences only occur in the regime where the bias ϵ_0 is below or around the energy scale given by ω_0. In the panels the exact ground-state energies E_g^{ex} are displayed.

In Figure 3.2 the ground-state energy E_g^{FE} obtained from the form-invariant flow - given by the set of equations (3.18) - is shown relative to the exact ground-state energy E_g^{ex} for two different tunnel-matrix elements $\Delta_0 = 0.5\omega_0$ (left hand side) and $\Delta_0 = 1.5\omega_0$ (right hand side). Drastic deviations from the exact result are seen in the regime $\epsilon_0 > \omega_0$. This means that the neglected operator $\mathcal{O}_1$ of Eq. (3.10) becomes relevant and has to be taken into account.

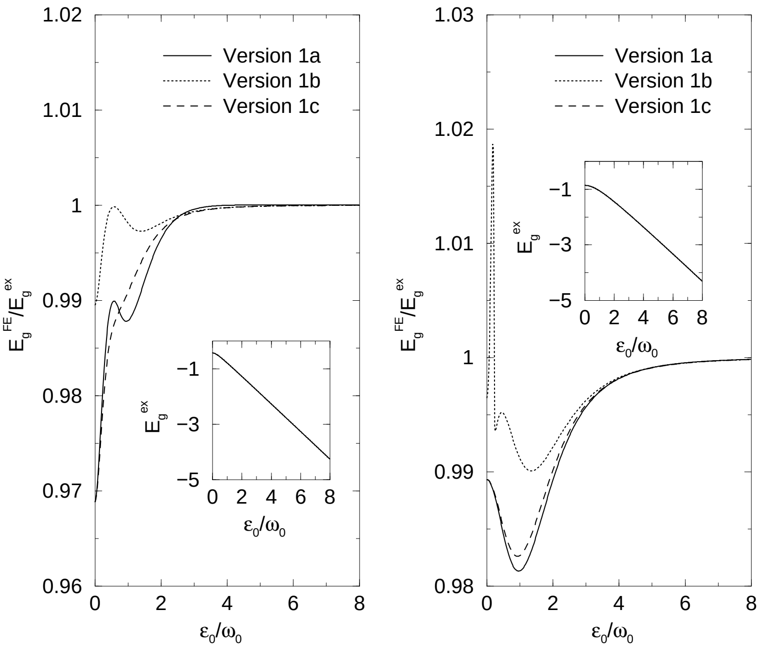

Figure 3.1.: The ground-state energy E_g^{FE} obtained by different canonical generators for the un-shifted bosonic representation for $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel.

Redefining $\mathcal{O}_1 \equiv \sigma_x\kappa_1 : (b+b^\dagger)^2 :$, the commutator $[\eta, \mathcal{O}_1]$ yields[4]

$$[\eta, \mathcal{O}_1] = 2\sigma_z\eta^{y,0}\kappa_1 : (b+b^\dagger)^2 : +2\sigma_z\eta^y\kappa_1(: (b+b^\dagger)^3 : +2\langle(b+b^\dagger)^2\rangle : (b+b^\dagger) :) \\ + 2i\sigma_y\eta^z\kappa_1 : (b-b^\dagger)(b+b^\dagger)^2 : \quad . \tag{3.44}$$

We want to first neglect the trilinear operators and the bilinear operator of type $\mathcal{O}_2$ (see Eq. (3.10)). Thus only considering the term linear in the bosonic operators, the extended Flow Equations read ($f = 1$ and $1_n \equiv 1 + 2n$)

$$\begin{aligned} &\partial_\ell\Delta = -\Delta\lambda^{z2}1_n + \Delta\epsilon^2 \quad , \quad \partial_\ell\epsilon = -\epsilon\Delta^2 \quad , \quad \partial_\ell\kappa_1 = \Delta\lambda^{z2}/2 \\ &\partial_\ell\lambda^z = \lambda^z(\Delta^2 - \omega_0^2) + 4\lambda^z\Delta\kappa_1 1_n \quad , \quad \partial_\ell E = -\omega_0\lambda^{z2}f/2 \quad . \end{aligned} \tag{3.45}$$

We will refer to this set of Flow Equations as Version 1d$'$.

To see if this improvement is systematic we will now include also the correction that comes from the neglected operator of type $\mathcal{O}_2$. Redefining $\mathcal{O}_2 \equiv \sigma_z\kappa_2 : (b+b^\dagger)^2 :$, we obtain similar commutator relations for $[\eta, \mathcal{O}_2]$ as we got in Eq. (3.44):

$$[\eta, \mathcal{O}_2] = -2\sigma_x\eta^{y,0}\kappa_2 : (b+b^\dagger)^2 : -2\sigma_x\eta^y\kappa_2(: (b+b^\dagger)^3 : +2\langle(b+b^\dagger)^2\rangle : (b+b^\dagger) :) \\ - 2i\sigma_y\eta^z\kappa_2 : (b-b^\dagger)(b+b^\dagger)^2 : \tag{3.46}$$

[4] For the normal ordering procedure see Appendix A.

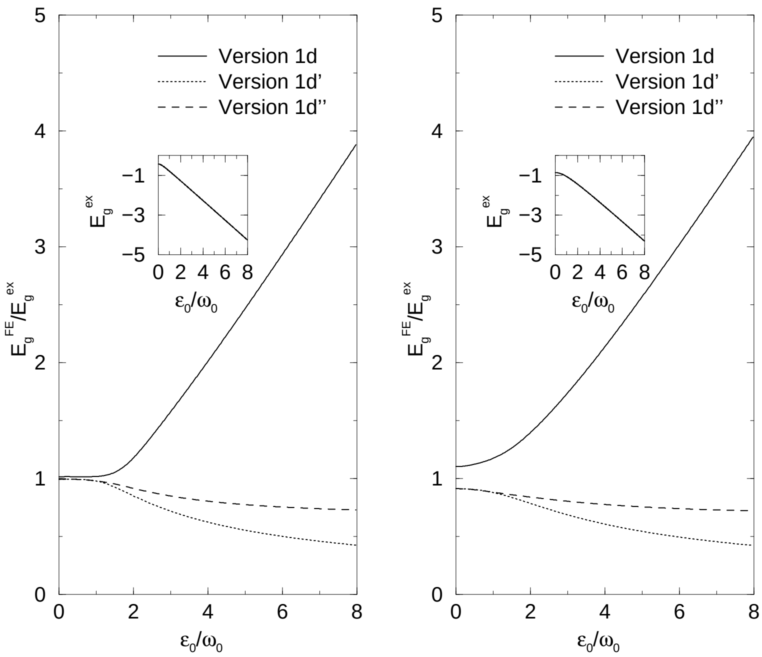

Figure 3.2.: The ground-state energy E_g^{FE} obtained from the form-invariant flow for $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel. The primed versions are including the flow of the neglected operators $\mathcal{O}_1$ and $\mathcal{O}_2$ (see text).

The effect of including $\mathcal{O}_2$ is that the conditions for the constants of the generator that assure the form-invariance of the Hamiltonian slightly change, see Eq. (3.17). The Flow Equations read ($f = 1$)

$$\begin{aligned}
\partial_\ell \Delta &= -\Delta \lambda^{z2} 1_n + \Delta\epsilon(\epsilon + 4\kappa_2) \quad , \quad \partial_\ell \epsilon = -(\epsilon + 4\kappa_2)\Delta^2 \\
\partial_\ell \lambda^z &= \lambda^z(\Delta^2 - \omega_0^2) + 4\lambda^z \Delta\kappa_1 1_n \quad , \quad \partial_\ell E = -\omega_0 \lambda^{z2} f/2 \\
\partial_\ell \kappa_1 &= \Delta\lambda^{z2}/2 - \Delta(\epsilon + 4\kappa_2)\kappa_2 \quad , \quad \partial_\ell \kappa_2 = \Delta(\epsilon + 4\kappa_2)\kappa_1
\end{aligned} \tag{3.47}$$

We will refer to this set of Flow Equations as Version 1d$''$.

In Figure 3.2 one sees that the extended Flow Equations yield a systematic improvement ranging over the whole parameter space. Nevertheless, the agreement with the exact result remains rather poor for $\epsilon > \omega_0$. Only if one considers the renormalization of the bath mode ω_0 one will obtain results within a few percent relative error over the whole parameter range.

We now turn to the Flow Equations based on the shifted bosonic modes given in subsection 3.1.2. Again the ground-state energy is determined by means of Flow Equations governed by the different canonical generators. They still depend on the

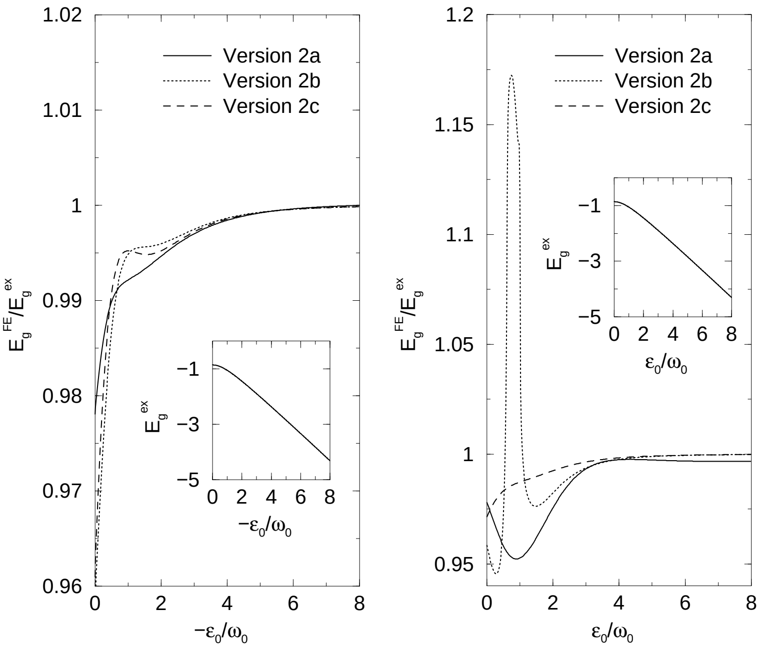

Figure 3.3.: The ground-state energy E_g^{FE} obtained by different canonical generators for the shifted bosonic representation for $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ and $\delta = -\lambda^z/\omega_0$ as a function of a negative (left hand side) and positive bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel

expectation value of the fermionic operators, or equivalently on the expectation value of the Pauli spin matrices. In Figure 3.3 the results are shown for $\langle c_1^\dagger c_1 \rangle = 1/2$ or equivalently $\langle \sigma_z \rangle = 0$ for all ℓ with the initial tunnel-matrix element $\Delta_0 = 1.5\omega_0$. The left and right hand side displays the results for negative and positive bias ϵ_0 respectively.

One obvious short-come of the Flow Equations of the shifted modes is that they are not invariant with respect to the sign of the initial bias ϵ_0. For negative bias the results are quantitatively better and more systematic. This can be understood since a negative bias induces the occupation of the fermionic state $i = 1$, which is the distinguished state of the initial Hamiltonian (3.2).

Providing a negative bias, the Flow Equations of the shifted representation yield better results than the ones based on the un-shifted representation shown on the right hand side of Figure 3.1.

Finally, we will investigate the dependence of the ground-state energy on the specific choice of the fermionic expectation values. On the left side of Figure 3.4 the expectation value was chosen to be ℓ-dependent and given by $1 - 2\langle c_1^\dagger c_1 \rangle = -\epsilon/\sqrt{\Delta^2 + \epsilon^2}$ with $\delta = -2\langle c_1^\dagger c_1 \rangle \lambda^z/\omega_0$. On the right side of Figure 3.4, the expectation values were chosen according to the extended truncation scheme given in Eq. (3.42) with

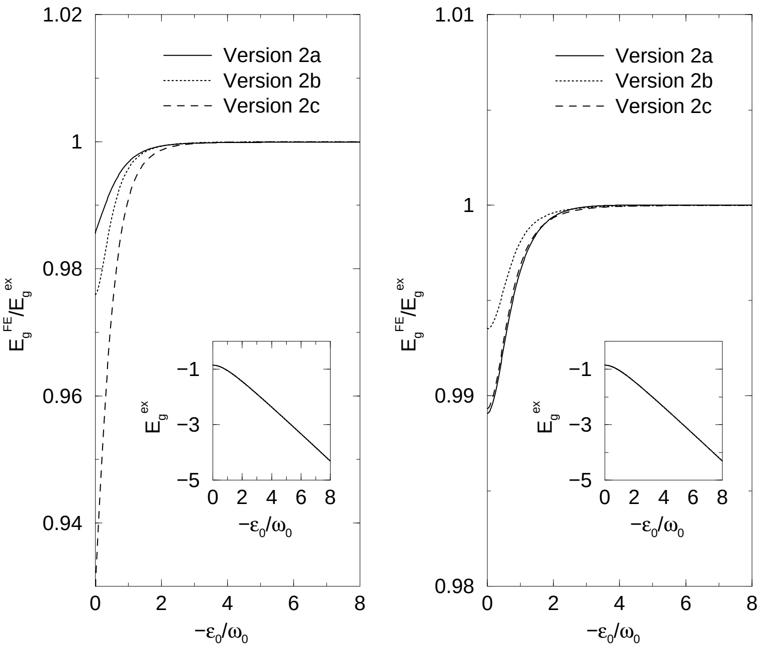

Figure 3.4.: The ground-state energy E_g^{FE} obtained by different canonical generators for the shifted bosonic representation for $\Delta_0/\omega_0 = 1.5$ and $\lambda_0/\omega_0 = 1$ with $\delta = -2\langle c_1^\dagger c_1\rangle\lambda^z/\omega_0$ (left) and $\delta = \lambda^e/\omega_0 + \langle\sigma_x\rangle\lambda^x/\omega_0 - 2\langle c_1^\dagger c_1\rangle\lambda^z/\omega_0$ and ℓ-dependent expectation values determined according to the corresponding truncation schemes (see text) as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel.

$\delta = \lambda^e/\omega_0 + \langle\sigma_x\rangle\lambda^x/\omega_0 - 2\langle c_1^\dagger c_1\rangle\lambda^z/\omega_0$.

Comparing the results that were obtained for different choices of the fermionic expectation values, one sees a systematic improvement if one includes more terms in the evaluation of the bosonic shift δ. The reference from the system back to the "bath" by including system properties in the normal ordering procedure thus stabilizes the flow of the parameters.

3.2. Flow of Observables

We will now investigate the flow of observables. First we will set up the Flow Equations for the Pauli spin matrices based on the un-shifted and shifted representation respectively. In order to characterize the quality of the Flow Equations sum rules are derived expressing the fact that $\sigma_i^2 = 1$ for all ℓ with $i = x, y, z$. As will be pointed out in the end of this section, these sum rules are somehow misleading. We will therefore also compare the Flow Equation results with the numerically exact fixed point of the operator flow. To so so we will give a unique decomposition of the fixed point operator into a basis of normal ordered bosonic operators.

3.2.1. Flow Equations for Un-shifted Mode

The Flow Equations for the Pauli spin matrices do not close and one thus needs a suitable truncation scheme. The i-component of the Pauli spin matrices as a function of the flow parameter ℓ shall be given by

$$\begin{aligned} \sigma_i(\ell) &= g_i(\ell)\sigma_x + h_i(\ell)\sigma_z + f_i(\ell) \\ &+ \sigma_x\chi^{x,i}(b+b^\dagger) + i\sigma_y\chi^{y,i}(b-b^\dagger) + \sigma_z\chi^{z,i}(b+b^\dagger) \quad , \end{aligned} \tag{3.48}$$

with $i = x, z$ and the flow of the y-component of the Pauli spin matrices by

$$i\sigma_y(\ell) = g_y(\ell)i\sigma_y + \sigma_x\chi^{x,y}(b-b^\dagger) + \sigma_z\chi^{z,y}(b-b^\dagger) \quad . \tag{3.49}$$

These are the most general expansions up to linear bosonic operators that can evolve from the Pauli spin matrices under Flow Equations, i.e. from $\sigma_i(\ell=0) = \sigma_i$.
The commutator $[\eta, \sigma_i]$ with $i = x, z$ yields the following contributions:

$$\begin{aligned} [\eta^{0,y}, \sigma_i(\ell)] &= 2\sigma_z g_i \eta^{0,y} - 2\sigma_x h_i \eta^{0,y} + 2\sigma_z\eta^{0,y}\chi^{x,i}(b+b^\dagger) \\ &- 2\sigma_x\eta^{0,y}\chi^{z,i}(b+b^\dagger) \end{aligned} \tag{3.50}$$

$$[\eta^{e}, \sigma_i(\ell)] = 2\sigma_x\eta^e\chi^{x,i} + 2\sigma_z\eta^e\chi^{z,i} \tag{3.51}$$

$$\begin{aligned} [\eta^{x}, \sigma_i(\ell)] &= -2i\sigma_y h_i\eta^x(b-b^\dagger) + 2\eta^x\chi^{x,i} - 2\sigma_z\eta^x\chi^{y,i}(b-b^\dagger)^2 \\ &- i\sigma_y\eta^x\chi^{z,i}\{(b-b^\dagger),(b+b^\dagger)\} \end{aligned} \tag{3.52}$$

$$\begin{aligned} [\eta^{y}, \sigma_i(\ell)] &= 2\sigma_z g_i\eta^y(b+b^\dagger) - 2h_i\sigma_x\eta^y(b+b^\dagger) \\ &+ 2\sigma_z\eta^y\chi^{x,i}(b+b^\dagger)^2 + 2\eta^y\chi^{y,i} - 2\sigma_x\eta^y\chi^{z,i}(b+b^\dagger)^2 \end{aligned} \tag{3.53}$$

$$\begin{aligned} [\eta^{z}, \sigma_i(\ell)] &= 2i\sigma_y g_i\eta^z(b-b^\dagger) + i\sigma_y\eta^z\chi^{x,i}\{(b-b^\dagger),(b+b^\dagger)\} \\ &+ 2\sigma_x\eta^z\chi^{y,i}(b-b^\dagger)^2 + 2\eta^z\chi^{z,i} \end{aligned} \tag{3.54}$$

The commutator $[\eta, i\sigma_y]$ is given by:

$$[\eta^{0,y}, \sigma_y(\ell)] = 2\sigma_z\eta^{0,y}\chi^{x,y}(b-b^\dagger) - 2\sigma_x\eta^{0,y}\chi^{z,y}(b-b^\dagger) \tag{3.55}$$

$$[\eta^{x}, \sigma_y(\ell)] = -2\sigma_z g_y\eta^x(b-b^\dagger) - 2i\sigma_y\eta^x\chi^{z,y}(b-b^\dagger)^2 \tag{3.56}$$

$$[\eta^{y}, \sigma_y(\ell)] = \sigma_z\eta^y\chi^{x,y}\{(b+b^\dagger),(b-b^\dagger)\} - \sigma_x\eta^y\chi^{z,y}\{(b+b^\dagger),(b-b^\dagger)\} \tag{3.57}$$

$$[\eta^{z}, \sigma_y(\ell)] = 2\sigma_x g_y\eta^z(b-b^\dagger) + 2i\sigma_y\eta^z\chi^{x,y}(b-b^\dagger)^2 \tag{3.58}$$

To understand which combinations of operators can transform into one another, we give a list of operators and their behaviour with respect to parity transformation (P) and Hermitian conjugation (H) ($x \equiv (b + b^\dagger)$, $p \equiv (b - b^\dagger)$) :

	1	σ_x	$i\sigma_y$	σ_z	x	p	$\sigma_x x$	$\sigma_x p$	$i\sigma_y x$	$i\sigma_y p$	$\sigma_z x$	$\sigma_z p$
P	+	+	−	−	+	−	−	−	+	+	+	+
H	+	+	−	+	+	−	+	−	−	+	+	−

Neglecting normal ordered bilinears one obtains the following coupled differential equations for the i-component of the Pauli spin matrices with $i = x, z$:

$$\partial_\ell g_i = -2h_i\eta^{0,y} + 2\eta^e\chi^{x,i} - 2\eta^z\chi^{y,i}(1+2n) - 2\eta^y\chi^{z,i}(1+2n) \tag{3.59}$$

$$\partial_\ell h_i = 2g_i\eta^{0,y} + 2\eta^y\chi^{x,i}(1+2n) + 2\eta^x\chi^{y,i}(1+2n) + 2\eta^e\chi^{z,i} \tag{3.60}$$

$$\partial_\ell f_i = 2\eta^x\chi^{x,i} + 2\eta^y\chi^{y,i} + 2\eta^z\chi^{z,i} \tag{3.61}$$

$$\partial_\ell\chi^{x,i} = -2h_i\eta^y - 2\eta^{0,y}\chi^{z,i} \quad , \quad \partial_\ell\chi^{y,i} = 2g_i\eta^z - 2h_i\eta^x \tag{3.62}$$

$$\partial_\ell\chi^{z,i} = 2g_i\eta^y + 2\eta^{0,y}\chi^{x,i} \tag{3.63}$$

The Flow Equations for the y-component read:

$$\partial_\ell g_y = -2\eta^z\chi^{x,y}(1+2n) + 2\eta^x\chi^{z,y}(1+2n) \tag{3.64}$$

$$\partial_\ell\chi^{x,y} = 2g_y\eta^z - 2\eta^{0,y}\chi^{z,y} \quad , \quad \partial_\ell\chi^{z,y} = -2g_y\eta^x + 2\eta^{0,y}\chi^{x,y} \tag{3.65}$$

Inserting the constants as obtained for the form-invariant flow of the Hamiltonian, the flow of σ_i for $i = x, z$ yields:

$$\partial_\ell g_i = \omega_0\lambda\chi^{y,i}(1+2n) + \Delta\lambda\chi^{z,i}(1+2n) - \epsilon\Delta h_i \tag{3.66}$$

$$\partial_\ell h_i = -\Delta\lambda\chi^{x,i}(1+2n) + \epsilon\Delta g_i \quad , \quad \partial_\ell f_i = -\Delta\lambda\chi^{y,i} - \omega_0\lambda\chi^{z,i} \tag{3.67}$$

$$\partial_\ell\chi^{x,i} = -\omega_0\lambda h_i - \epsilon\Delta\chi^{z,i} \quad , \quad \partial_\ell\chi^{y,i} = -\omega_0\lambda g_i \tag{3.68}$$

$$\partial_\ell\chi^{z,i} = -\Delta\lambda g_i + \epsilon\Delta\chi^{x,i} \tag{3.69}$$

Certain conservation laws should hold approximately since we are performing an approximate unitary transformation. First $\langle\sigma_i^2(\ell)\rangle = 1$ should hold for $i = x, y, z$. For $\epsilon = 0$ this relation holds exactly for all ℓ for $i = y, z$. For $i = x$ we obtain the relation $g_x^2 + f_x^2 + ((\chi^{y,x})^2 + (\chi^{z,x})^2)(1+2n) + 2g_x h_x - 2\chi^{y,x}\chi^{z,x} \approx 1$. Differentiating both sides by ℓ yields $\partial_\ell\langle\sigma_i^2(\ell)\rangle = 4h(\eta^y - \eta^z)(\chi^{y,x} - \chi^{z,x}) \approx 0$.

Other conservation relations follow from the commutator $[i\sigma_y(\ell), \sigma_z(\ell)] = -2\sigma_x(\ell)$.

We would like to comment on the constant term f_i appearing in the expansion of the Pauli spin matrices σ_i with $i = x, z$. This term seems to contradict the theorem of the invariance of the trace under unitary transformations. But since the trace of

$\sigma_i(\ell=0) = \sigma_i \otimes 1$, 1 being the identity of the bosonic Hilbert space, does not exist and since we also expand the Pauli spin matrices in a series of unbounded operators the above mentioned theorem does not hold anymore. To make sure that the constant term is indeed physical, one can truncate the Hilbert space by introducing the "bosonic" operator

$$b \to b_N = b\sqrt{(1 - b^\dagger b/N)} \quad , \tag{3.70}$$

with N being a positive integer. The truncated Hilbert space is now only spanned by N vectors $|\nu\rangle = (b^\dagger)^\nu/\sqrt{\nu!}|0\rangle$ with $\nu = 0...N-1$ and $b|0\rangle = 0$. For $N \to \infty$ we recover the bosonic Hilbert space. The above theorem is guaranteed due to the new, non-canonical commutation relation $[b_N, b_N^\dagger] = 1 - (1 + 2b^\dagger b)/N$ which obeys the cyclic invariance of the trace:[5]

$$\mathrm{tr}([b_N, b_N^\dagger]) = \sum_{\nu=0}^{N-1}(1 - \frac{1+2\nu}{N}) = 0 \tag{3.71}$$

The Flow Equations (3.66) - (3.69) now have to be extended to include the flow of the operator $b^\dagger b$ that appears in the commutator relation and that scales as $1/N$. The constant term f_i appears nevertheless and is governed by the same differential equation (3.61) as $N \to \infty$. Both terms together, the constant term f_i and the bosonic bilinear $b^\dagger b$, make sure that no trace is generated during the flow.

3.2.2. Flow Equations for Shifted Mode

We will now consider the Flow Equations based on the shifted representation of the bosonic modes. The truncation scheme for the Pauli spin matrices shall be given in Eqs. (3.48) and (3.49) and therefore also the commutators $[\eta, \sigma_i]$ with $i = x, y, z$ remain the same. But this time the neglected normal ordered bilinears are to be taken with respect to the shifted bosonic modes. Thus one obtains the following coupled differential equations for the i-component of the Pauli spin matrices with $i = x, z$:

$$\partial_\ell g_i = -2h_i\eta^{0,y} + 2\eta^e\chi^{x,i} - 2\eta^z\chi^{y,i}(1+2n) - 2\eta^y\chi^{z,i}(1+2n) + 2\eta^y\chi^{z,i}\delta^2 \tag{3.72}$$

$$\partial_\ell h_i = 2g_i\eta^{0,y} + 2\eta^y\chi^{x,i}(1+2n) + 2\eta^x\chi^{y,i}(1+2n) + 2\eta^e\chi^{z,i} - 2\eta^y\chi^{x,i}\delta^2 \tag{3.73}$$

$$\partial_\ell f_i = 2\eta^x\chi^{x,i} + 2\eta^y\chi^{y,i} + 2\eta^z\chi^{z,i} \tag{3.74}$$

$$\partial_\ell\chi^{x,i} = -2h_i\eta^y - 2\eta^{0,y}\chi^{z,i} + 4\eta^y\chi^{z,i}\delta \tag{3.75}$$

$$\partial_\ell\chi^{y,i} = 2g_i\eta^z - 2h_i\eta^x + 2\eta^x\chi^{z,i}\delta - 2\eta^z\chi^{x,i}\delta \tag{3.76}$$

$$\partial_\ell\chi^{z,i} = 2g_i\eta^y + 2\eta^{0,y}\chi^{x,i} - 4\eta^y\chi^{x,i}\delta \tag{3.77}$$

[5] See also Ref. [Jud63] for related commutator relations.

Again δ denotes the shift in the bosonic operator. The Flow Equations for the y-component are left unchanged with respect to the un-shifted version. They read:

$$\partial_\ell g_y = -2\eta^z\chi^{x,y}(1+2n) + 2\eta^x\chi^{z,y}(1+2n) \tag{3.78}$$

$$\partial_\ell\chi^{x,y} = 2g_y\eta^z - 2\eta^{0,y}\chi^{z,y} - 2\eta^y\chi^{z,y}\delta \quad , \quad \partial_\ell\chi^{z,y} = -2g_y\eta^{0,y}x + 2\eta^{0,y}\chi^{x,y} - 2\eta^y\chi^{x,y}\delta \tag{3.79}$$

If no approximation was made, $\sigma_i^2(\ell) = 1$ would hold for all ℓ and $i = x, y, z$. Taking the expectation value with respect to the bilinear Hamiltonian of the shifted modes the relation should hold approximately for $i = x, z$:

$$\begin{aligned}\langle\sigma_i^2(\ell)\rangle &= g_i^2 + h_i^2 + f_i^2 + (\chi^{x,i}\chi^{x,i} + \chi^{y,i}\chi^{y,i} + \chi^{z,i}\chi^{z,i})(1+2n)\\ &+ 2(g_i\langle\sigma_x\rangle + h_i\langle\sigma_z\rangle)f_i + 2(\chi^{x,i}\langle\sigma_z\rangle - \chi^{z,i}\langle\sigma_x\rangle)\chi^{y,i}\\ &+ (\chi^{x,i}\chi^{x,i} + \chi^{z,i}\chi^{z,i})\delta^2 - 2((g+\langle\sigma_x\rangle f)\chi^{x,i} + (h+\langle\sigma_z\rangle f)\chi^{z,i})\delta\\ &\approx 1\end{aligned} \tag{3.80}$$

For the y-component we obtain:

$$\langle\sigma_y^2(\ell)\rangle = g_y^2 + (\chi^{x,y}\chi^{x,y} + \chi^{z,y}\chi^{z,y})(1+2n) \approx 1 \tag{3.81}$$

Other conservation relations follow from the commutator $[i\sigma_y(\ell), \sigma_z(\ell)] = 2i\sigma_x(\ell)$.

Instead of the ansatz of the operator flow given in Eq. (3.48) one can define the observable flow with respect to the shifted mode. The i-component of the Pauli spin matrices as a function of the flow parameter ℓ shall thus be given by

$$\begin{aligned}\sigma_i(\ell) &= g_i(\ell)\sigma_x + h_i(\ell)\sigma_z + f_i(\ell)\\ &+ \sigma_x\chi^{x,i}(\bar{b} + \bar{b}^\dagger) + i\sigma_y\chi^{y,i}(\bar{b} - \bar{b}^\dagger) + \sigma_z\chi^{z,i}(\bar{b} + \bar{b}^\dagger) \quad ,\end{aligned} \tag{3.82}$$

with $i = x, z$ and $\bar{b} = b + \delta$. The ansatz for σ_y is left unchanged.

The commutator $[\eta, \sigma_i]$ is related to the corresponding commutator given above. We will therefore only present the resulting Flow Equations ($1_n \equiv (1+2n)$):

$$\partial_\ell g_i = -2h_i\eta^{0,y} + 2\eta^e\chi^{x,i} - 2\eta^z\chi^{y,i}1_n - 2\eta^y\chi^{z,i}1_n + 2h_i\eta^y\delta - \chi^{x,i}\partial_\ell\delta \tag{3.83}$$

$$\partial_\ell h_i = 2g_i\eta^{0,y} + 2\eta^y\chi^{x,i}1_n + 2\eta^x\chi^{y,i}1_n + 2\eta^e\chi^{z,i} - 2g_i\eta^y\delta - \chi^{z,i}\partial_\ell\delta \tag{3.84}$$

$$\partial_\ell f_i = 2\eta^x\chi^{x,i} + 2\eta^y\chi^{y,i} + 2\eta^z\chi^{z,i} \tag{3.85}$$

$$\partial_\ell\chi^{x,i} = -2h_i\eta^y - 2\eta^{0,y}\chi^{z,i} + 2\eta^y\chi^{z,i}\delta \quad , \quad \partial_\ell\chi^{y,i} = 2g_i\eta^z - 2h_i\eta^x \tag{3.86}$$

$$\partial_\ell\chi^{z,i} = 2g_i\eta^y + 2\eta^{0,y}\chi^{x,i} - 2\eta^y\chi^{x,i}\delta \tag{3.87}$$

Notice that in the first two equations of the above set contributions of the form $\chi^{i,i}\partial_\ell\delta$ appear, that stem from the ℓ-dependence of $\bar{b}$. The approximate sum rule now reads

$$\begin{aligned}\langle\sigma_i^2(\ell)\rangle &= g_i^2 + h_i^2 + f_i^2 + (\chi^{x,i}\chi^{x,i} + \chi^{y,i}\chi^{y,i} + \chi^{z,i}\chi^{z,i})1_n\\ &+ 2(g_i\langle\sigma_x\rangle + h_i\langle\sigma_z\rangle)f_i + 2(\chi^{x,i}\langle\sigma_z\rangle - \chi^{z,i}\langle\sigma_x\rangle)\chi^{y,i} \approx 1 \quad .\end{aligned} \tag{3.88}$$

3.2.3. Higher Orders

In the expansion of the Pauli spin matrices in Eqs. (3.48) and (3.49) we have neglected all generated operators with more than one bosonic operator. In order to confirm that the expansion of the Pauli spin matrices in normal ordered bosonic operators is indeed systematic we will now upgrade our expansion and also include:

- all generated operators up to two normal ordered bosonic operators
- all generated operators up to three normal ordered bosonic operators

In the following normal ordering shall be defined with respect to the bilinear Hamiltonian of the un-shifted mode. We will therefore only consider the extensions of the Flow Equations of subsection 3.2.1.

The first extension $\sigma_z^{new,2}$ includes the following terms, where we introduce the abbreviations $x \equiv b + b^\dagger$ and $p \equiv b - b^\dagger$ and where we also confine ourself to the discussion of σ_z in order to be able to drop one index:

$$\begin{aligned}\sigma_z^{new,2} &= \chi^1 x + \sigma_x \psi^{x,+} : x^2 : + i\sigma_y \psi^{y,+} : xp : \\ &+ \sigma_z \psi^{z,+} : x^2 : + \sigma_x \psi^{x,-} : p^2 : + \sigma_z \psi^{z,-} : p^2 :\end{aligned} \tag{3.89}$$

Note that also a term linear in the bosonic operators is created. The second extension $\sigma_z^{new,3}$ consists of the following terms:

$$\begin{aligned}\sigma_z^{new,3} &= \psi^{1,+} : x^2 : + \psi^{1,-} : p^2 : + \sigma_x \varphi^{x,+} : x^3 : + i\sigma_y \varphi^{y,+} : x^2 p : \\ &+ \sigma_z \varphi^{z,+} : x^3 : + \sigma_x \varphi^{x,-} : xp^2 : + i\sigma_y \varphi^{y,-} : p^3 : + \sigma_z \psi^{z,-} : xp^2 :\end{aligned} \tag{3.90}$$

Since the basic objects of our expansion are normal ordered operators we will give some (anti-)commutation rules which are helpful to evaluate the commutator $[\eta, \sigma_z]$ (see also Appendix A):

$$[x, : p^n x^m :] = -2n : p^{n-1} x^m : \quad , \quad [p, : p^n x^m :] = 2m : p^n x^{m-1} : \tag{3.91}$$

$$\{x, : p^n x^m :\} = 2 : p^n x^{m+1} : + 2m : p^n x^{m-1} : 1_n \tag{3.92}$$

$$\{p, : p^n x^m :\} = 2 : p^{n+1} x^m : - 2n : p^{n-1} x^m : 1_n \tag{3.93}$$

The commutator of two tensor products of the fermionic and bosonic Hilbert space can be written as $[oB, o'B'] = \{o, o'\}[B, B']/2 + [o, o']\{B, B'\}/2$ which is a useful identity if the anti-commutator $\{o, o'\}$ vanishes ($o, o' \in \mathcal{H}_e$, $B, B' \in \mathcal{H}_b$).

We will not write here the commutator $[\eta, \sigma_z]$ explicitly but only account for the additional terms that appear with respect to the previous Flow Equations of Eq. (3.59) - (3.63) and for the Flow Equations of the new parameters. For the first extension this yields:

$$\partial_\ell g_z = ... + 2\eta^x \chi^1 \quad , \quad \partial_\ell h_z = ... + 2\eta^z \chi^1 \tag{3.94}$$
$$\partial_\ell \chi^x = ... - 2\eta^z \psi^y 1_n - 4\eta^y \psi^{z,+} 1_n \tag{3.95}$$
$$\partial_\ell \chi^y = ... - 4\eta^z \psi^{x,-} 1_n + 4\eta^x \psi^{z,-} 1_n \tag{3.96}$$
$$\partial_\ell \chi^z = ... + 2\eta^x \psi^y 1_n + 4\eta^y \psi^{x,+} 1_n \tag{3.97}$$
$$\partial_\ell \chi^1 = 4\eta^z \psi^{z,+} - 2\eta^y \psi^y + 4\eta^x \psi^{x,+} \tag{3.98}$$
$$\partial_\ell \psi^{x,+} = -2\eta^y \chi^z - 2\eta^{0,y} \psi^{z,+} \tag{3.99}$$
$$\partial_\ell \psi^y = 2\eta^z \chi^x - 2\eta^x \chi^z \tag{3.100}$$
$$\partial_\ell \psi^{z,+} = 2\eta^y \chi^x + 2\eta^{0,y} \psi^{x,+} \tag{3.101}$$
$$\partial_\ell \psi^{x,-} = 2\eta^z \chi^y - 2\eta^{0,y} \psi^{z,-} \tag{3.102}$$
$$\partial_\ell \psi^{z,-} = -2\eta^x \chi^y + 2\eta^{0,y} \psi^{x,-} \tag{3.103}$$

Additional contribution relative to the previous Flow Equations coming from $\sigma_z^{new,3}$ read:

$$\partial_\ell \chi^x = ... + 4\eta^x \psi^{1,+} \ , \ \partial_\ell \chi^y = ... - 4\eta^y \psi^{1,-} \ , \ \partial_\ell \chi^z = ... + 4\eta^z \psi^{1,+} \tag{3.104}$$
$$\partial_\ell \psi^{x,+} = ... - 2\eta^z \varphi^{y,+} 1_n - 6\eta^y \varphi^{z,+} 1_n \tag{3.105}$$
$$\partial_\ell \psi^y = ... - 4\eta^z \varphi^{x,-} 1_n + 4\eta^x \varphi^{z,-} 1_n \tag{3.106}$$
$$\partial_\ell \psi^{z,+} = ... + 2\eta^x \varphi^{y,+} 1_n + 6\eta^y \varphi^{x,+} 1_n \tag{3.107}$$
$$\partial_\ell \psi^{x,-} = ... - 6\eta^z \varphi^{y,-} 1_n - 4\eta^y \varphi^{z,-} 1_n \tag{3.108}$$
$$\partial_\ell \psi^{z,-} = ... + 6\eta^x \varphi^{y,-} 1_n + 4\eta^y \varphi^{x,-} 1_n \tag{3.109}$$

The Flow Equations for the new parameter of $\sigma_z^{new,3}$ yield:

$$\partial_\ell \psi^{1,+} = 6\eta^z \varphi^{z,+} + 2\eta^y \varphi^{y,+} + 6\eta^x \varphi^{x,+} \tag{3.110}$$
$$\partial_\ell \psi^{1,-} = 2\eta^z \varphi^{z,-} + 6\eta^y \varphi^{y,-} + 2\eta^x \varphi^{x,-} \tag{3.111}$$
$$\partial_\ell \varphi^{x,+} = -2\eta^y \psi^{z,+} - 2\eta^{0,y} \varphi^{z,+} \tag{3.112}$$
$$\partial_\ell \varphi^{y,+} = 2\eta^z \psi^{x,-} - 2\eta^x \psi^{z,-} \tag{3.113}$$
$$\partial_\ell \varphi^{z,+} = 2\eta^y \psi^{z,+} + 2\eta^{0,y} \varphi^{x,+} \tag{3.114}$$
$$\partial_\ell \varphi^{x,-} = 2\eta^z \psi^y - 2\eta^y \psi^{z,-} - 2\eta^{0,y} \varphi^{z,-} \tag{3.115}$$
$$\partial_\ell \varphi^{y,-} = 2\eta^z \psi^{x,+} - 2\eta^x \psi^{z,+} \tag{3.116}$$
$$\partial_\ell \varphi^{z,-} = -2\eta^x \psi^y + 2\eta^y \psi^{x,-} + 2\eta^{0,y} \varphi^{x,-} \tag{3.117}$$

3.2.4. Numerical Results

We are now set to compare the results for the operator flow of the different approaches. Moreover, we will be able to compare them with the exact solution. How this is done will be outlined in the beginning of this subsection.

We recall that the Rabi Hamiltonian with only one mode is given by

$$H = -\frac{\Delta_0}{2}\sigma_x + \frac{\epsilon_0}{2}\sigma_z + \omega_0 b^\dagger b + \sigma_z \frac{\lambda_0}{2}(b + b^\dagger) + E_0 \quad . \tag{3.118}$$

Since there is only one mode present a numerical diagonalization is feasible by truncating the bosonic Hilbert space after n bosonic excitations with $n = 10$ say. In order to compare the results with the Flow Equation approach not only on the spectral but also on the operator level we will diagonalize the Hamiltonian in this basis in which the corresponding H_0 of the Flow Equation approach is diagonal.

Let $H_\mathrm{D} = UHU^\dagger$ be the diagonal Hamiltonian, then $\sigma_i^* = U\sigma_i U^\dagger$ is the operator to be compared with $\sigma_i(\ell = \infty)$ stemming from the Flow Equation approach, with $i = x, y, z$. To do so we will decompose σ_i^* in a set of operators which are created by the corresponding Flow Equations.

If one uses an expansion which is *normal ordered* in the bosonic operators the decomposition can be obtained numerically without any approximation.[6] The reason for this is that the bosonic ladder operators cannot compensate each other and then act on lower bosonic subspaces. To make this more explicit the general matrix structure of a normal ordered operator consisting of N bosonic operators is shown on the left hand side of Figure 3.5, taking $\{|\nu\rangle\}$ as basis with $|\nu\rangle \equiv (b^\dagger)^\nu/\sqrt{\nu!}|0\rangle$ and $b|0\rangle = 0$, ν being a positive integer. The dark area contains non-zero entries whereas the white area contains no entries. In case of a non-normal ordered operator the white, upper left triangle would also contain entries.

As an explicit choice of the operator basis for real symmetric operators like σ_x and σ_z we choose the set $\{o : (b + b^\dagger)^n(b - b^\dagger)^{2m} :, o' : (b + b^\dagger)^{n'}(b - b^\dagger)^{2m'+1} :\}$, where $o = 1, \sigma_x, \sigma_z$ and $o' = i\sigma_y$. The operator basis for real antisymmetric operators is obtained by interchanging o and o'. In the following we will only consider the flow of real symmetric operators. The results also hold for the real antisymmetric case.

We want to decompose a real symmetric operator into a set of finite operators. Considering all operators of the basis given above with less or equal than $2N$-bosonic operators we obtain a finite basis of $3\sum_{m=0}^{N}\sum_{n=0}^{2(N-m)} + \sum_{m'=0}^{N}\sum_{n'=1}^{2(N-m')} = (N+1)(4N+3)$ operators. Summing up the independent matrix elements which are uniquely determined by the normal ordered operators containing up to $2N$ bosonic modes, we obtain $\sum_{n=0}^{N} 2(4n + 1) + 1 = 4(N + 1)N + 3(N + 1) = (N + 1)(4N + 3)$. These independent matrix elements are located at the upper left triangle of the matrix, indicated as dark area on the right hand side of Figure 3.5.

[6] We neglect errors coming from the truncation of the Hilbert space.

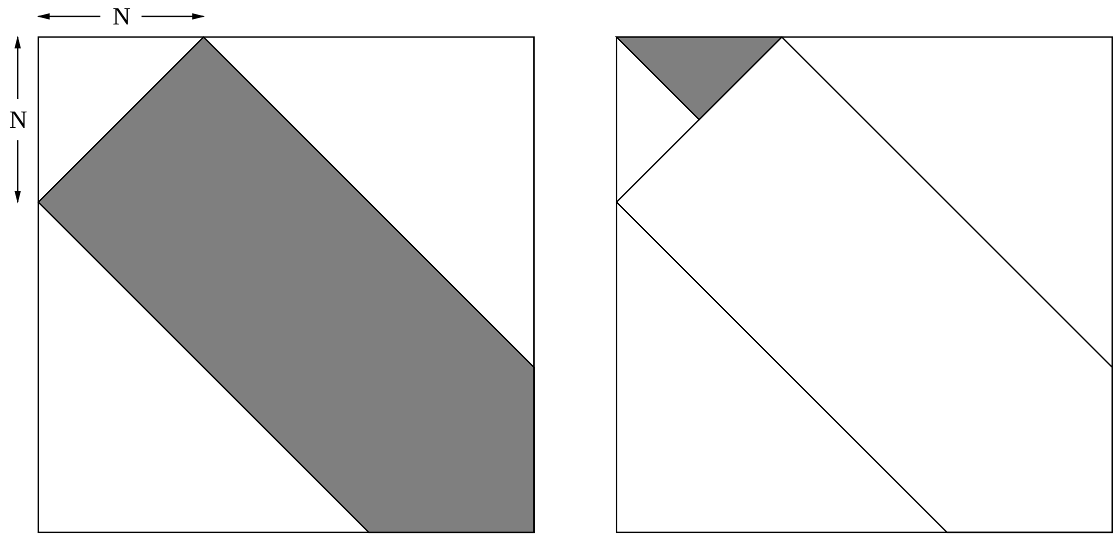

Figure 3.5.: Left hand side: Matrix structure of a normal ordered bosonic operator consisting of N bosonic operators with respect to the canonical basis (see text). The dark area indicates non-zero entries. Right hand side: The dark area indicates the matrix elements of an arbitrary matrix which are uniquely determined by normal ordered operators consisting of up to a certain number of bosonic operators (see text).

In order to complete the discussion we also consider all operators with less or equal than $(2N+1)$-bosonic operators. We then obtain a basis with $3\sum_{m=0}^{N}\sum_{n=0}^{2(N-m)+1}+\sum_{m'=0}^{N}\sum_{n'=0}^{2(N-m')} = (N+1)(4N+7)$ operators. Summing up the independent matrix elements which are uniquely determined by the normal ordered operators containing up to $2N+1$ bosonic modes, we obtain $\sum_{n=0}^{N} 2(4n+3)+1 = 4(N+1)N+7(N+1) = (N+1)(4N+7)$.

We thus obtain the same number of independent matrix elements and basis "vectors". This confirms that our basis is complete and linearly independent as we take $N \to \infty$. Secondly, this shows that the first $(N+1)(4N+3)$ coordinates of a real symmetric operator with respect to a finite basis of operators up to $2N$ bosonic operators are left unchanged if one goes over to a finite basis including $2N+M$ bosonic operators $(M > 0)$.

We can thus *exactly* determine the coefficients of our basis up to any number of bosonic excitations N which σ_i^* is composed of. This shows that choosing a set of normal ordered bosonic operators as a basis yields a systematic approximation of any operator. If one is only interested in the system dynamics at low energies it thus suffices to consider only up to N bosonic modes with $N=2$ say.

To determine the coefficients numerically one has to work with a specific basis.

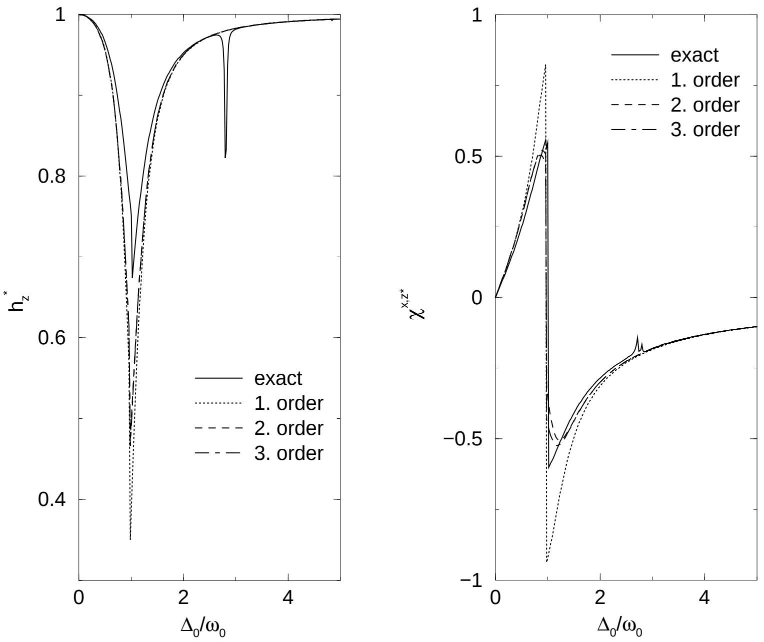

Figure 3.6.: The fixed point parameters $h_z^* \equiv h_z(\ell = \infty)$ (left hand side) and $\chi^{x,z*} \equiv \chi^{x,z}(\ell = \infty)$ stemming from the symmetric Flow Equations of Version 1a for $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ for different orders of truncation of the operator flow as a function of Δ_0. The solid lines resembles the exact result.

Up to now we have only specified the basis of the bosonic Hilbert space. Choosing $H_0 = -\frac{\Delta_0}{2}\sigma_x + \omega_0 b^\dagger b$ to be diagonal we are led to the basis $\{|e,\nu\rangle\}$ with the first quantum number $e = 0, 1$ denoting the eigenstates of σ_x and the second quantum number denoting the eigenstates of $b^\dagger b$.

Considering all operators with less or equal than $2N$-bosonic operators we end up to solve a linear equation $Ax = b$, with A being a quadratic matrix and x, b being vectors with dimensions $(N+1)(4N+3)$. The coefficients of the matrix A are obtained from the following matrix representations of normal ordered bosonic operators:

$$\langle e,\mu|o : (b+b^\dagger)^n (b-b^\dagger)^{2m} : |e',\nu\rangle = \langle e|o|e'\rangle \sum_{k=0}^{n} \binom{n}{k} \sum_{l=0}^{2m} \binom{2m}{l} (-1)^{2m-l}$$

$$\times\, \Theta(\nu-k-l) \sqrt{\frac{\mu!}{(N-k-l)!}} \sqrt{\frac{\nu!}{(N-k-l)!}} \delta_{\mu,\nu+n+2(m-k-l)} \qquad (3.119)$$

The vector b on the right hand side of the linear equation is given by the $(N+1)(4N+3)$ independent matrix elements, located at the dark area of the matrix of the right hand side of Figure 3.5.

We are now set to compare the fixed points of the operator flow obtained from

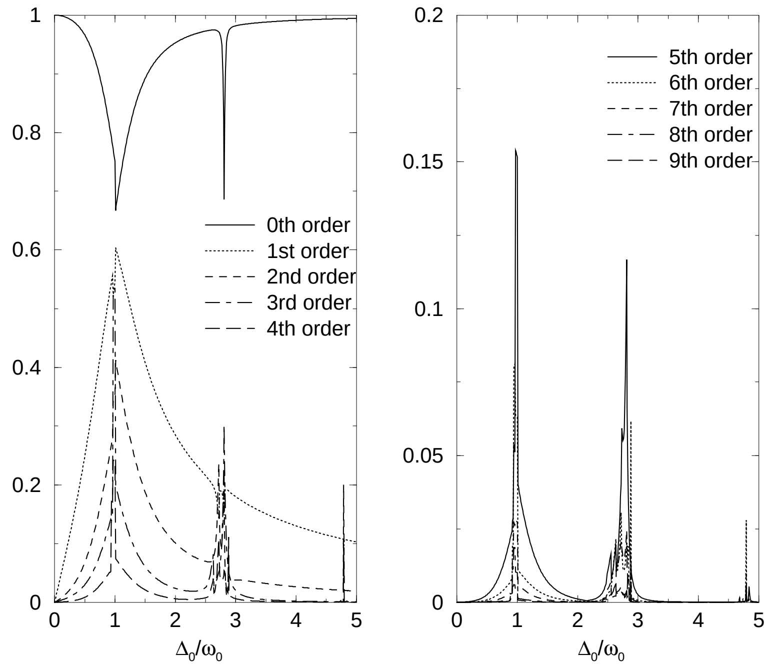

Figure 3.7.: The sum of the absolute values of the coefficients of all operators that consist of n bosonic operators (nth order) for $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ as function of Δ_0.

the Flow Equation approach with the exact results. We can also see from the exact solution if the expansion into normal ordered bosonic operators is preferable.

It turns out that the expansion into normal ordered operators is not unproblematic. Especially when the reflection symmetry is broken, i.e. $\epsilon_0 \neq 0$, the final values of the coefficients delicately depend on the initial parameters of the Hamiltonian. The reason for this is that the unperturbed states cross when the interaction is switched on and this effects the representation of the operator. The effect is enhanced by explicitly breaking certain symmetries.

We therefore limit our interest to the parameter regime where the reflection symmetry is not broken, i.e. $\epsilon_0 = 0$. If we choose the generator of Version 1a and consider the flow of the z-component of the Pauli spin matrices given in Eqs. (3.59) - (3.63), only two parameters h_z and $\chi^{x,z}$ are being renormalized. The final values $h_z^* \equiv h_z(\ell = \infty)$ and $\chi^{x,z*} \equiv \chi^{x,z}(\ell = \infty)$ are shown for the initial condition $\lambda_0/\omega_0 = 0.5$ in Figure 3.6, together with the results where we also included the flow of bilinear (2. order) and trilinear (3. order) bosonic operators, governed by Eqs. (3.94) - (3.103) and Eqs. (3.104) - (3.117).

The fixed point coefficients h_z^* and $\chi^{x,z*}$ agree with the exact solution unless the initial tunnel-matrix element Δ_0 is close to resonances, i.e. $\Delta_0 \approx \omega_0$ or $\Delta_0 \approx 3\omega_0$.[7]

[7]In Appendix C the Rabi model is treated in perturbation theory based on the exactly solvable

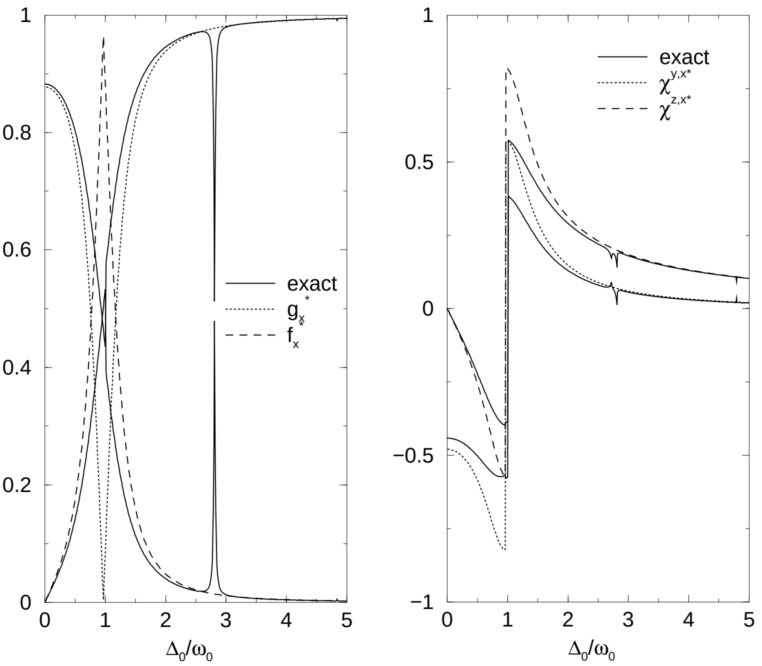

Figure 3.8.: The parameters $g_x^* \equiv g_x(\ell = \infty)$ and $f_x^* \equiv f_x(\ell = \infty)$ (left hand side) as well as $\chi^{y,x*} \equiv \chi^{y,x}(\ell = \infty)$ and $\chi^{z,x*} \equiv \chi^{z,x}(\ell = \infty)$ stemming from the symmetric Flow Equations of Version 1a for $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ as function of Δ_0. The solid lines resemble the analytic results.

The spike at $\Delta_0 \approx 3\omega_0$ cannot be accounted for by any of the solutions obtained via Flow Equations. But there is a significant improvement from the second order to the first order result close to the resonance at $\Delta_0 \approx \omega_0$ especially in the case of $\chi^{x,z*}$. The improvement from third to second order in the case of $\chi^{x,z*}$ is not as strong and the one particle parameter h_z^* is almost left unchanged.

To investigate the reason for these discrepancies we are going to employ the numerically exact solution and determine the expansion of the final operator $\sigma_z^* = U\sigma_z U^\dagger$ including up to nine bosonic operators. Instead of analyzing the graphs of all 115 coefficients we will consider the sum of the absolute values of the coefficients that belong to the operator class which consists of n bosonic operators (nth-order). The resulting nine graphs are shown in Figure 3.7. As can be seen, the second order still contributes to the fixed point operator considerably. Close to resonances even higher orders become important for the operator expansion. This explains why the fixed point parameter h_z^* is not sufficiently recovered by the Flow Equation approach even after including all terms up to three bosonic operators into the Flow Equations.

In Appendix C, the spikes of Figure 3.7 are related to degeneracies. The formalism

Jaynes-Cummings Model. In this context resonances are characterized by the vanishing of the energy denominator of the perturbative expansion.

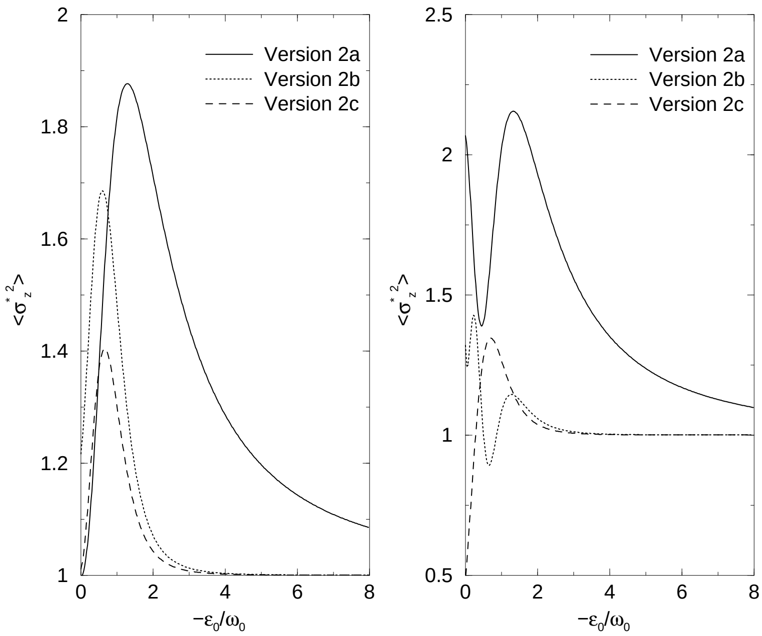

Figure 3.9.: The sum rule of $\sigma_z^* \equiv \sigma(\ell = \infty)$ for different versions of the Flow Equations for the shifted mode, employing the ansatz of the operator flow with the un-shifted mode (left hand side) and the ansatz of the operator flow with the shifted mode (right hand side) for $\Delta_0/\omega_0 = 1.5$ and $\lambda_0/\omega_0 = 1$ as function of the bias ϵ_0.

thus breaks down at these parameter configurations. This is related to the problem that occurs when diagonalizing the Hamiltonian which is, strictly speaking, also only possible for non-degenerate states.

In Figure 3.8, the results for the fixed point operator σ_x^* are shown as they follow from the Flow Equations of Version 1a with the initial conditions $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$. Four parameters $g_x^* \equiv g_x(\ell = \infty)$, $f_x^* \equiv f_x(\ell = \infty)$, $\chi^{y,x*} \equiv \chi^{y,x}(\ell = \infty)$, and $\chi^{z,x*} \equiv \chi^{z,x}(\ell = \infty)$ are generated during the flow. They show the same deficiencies with respect to the exact solution as the results of Figure 3.6. We want to mention that the constant term f_x^* is indeed generated, as can be seen from the exact expansion.

Let us conclude with a remark on the comparison of the operator flow with respect to the different versions of the Flow Equations, discussed in the previous section. Since most of the versions are based on different diagonal Hamiltonians H_0, a direct comparison of the fixed point parameters is troublesome. More reasonable would be to analyze the different sum rules. But this would have to be done with caution because of the following reason: Taking the initial parameters of the Hamiltonian as in Figure 3.6, the Flow Equations of Version 1a yield the exact sum rule $\langle \sigma_z^2 \rangle = h^2 + (\chi^{x,z})^2 = 1$ at $T = 0$ for all ℓ and independent of the initial tunnel-matrix element Δ_0. The sum rule is thus not sensitive to the deviations between the Flow Equation results and the exact solution, which become especially drastic close to resonances. We observe the situation that two errors are being canceled to yield the desired result. We therefore conclude that the sum rule cannot be a sufficient criterion for the quality of the operator flow.

With this caution in mind, we will close this section with a comparison of the sum rule originating from the Flow Equations of the shifted modes. In Figure 3.9 the sum rule of the fixed point operator $\sigma_z^* \equiv \sigma(\ell = \infty)$ is shown, employing the ansatz of the operator flow with the un-shifted mode of Eq. (3.48) (left hand side) and the ansatz with the shifted mode of Eq. (3.82) (right hand side) for $\Delta_0/\omega_0 = 1.5$ and $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0.[8]

Both *ansätze* yield rather poor results for $\epsilon_0/\omega_0 \leq 2$, even though the ansatz with the un-shifted mode of Eq. (3.48) appears to be preferable. Nevertheless, we will employ the shifted representation of the operator flow in the next chapters - involving a real bath consisting of an arbitrary number of modes - since this might treat the different modes more adequately.

[8]Notice that since Version 2c precedes a unitary transformation with respect to the fermionic Hilbert space, the same has to be done for the initial observable.

4. Spin-Boson Model

The most prominent dissipative quantum system is the Spin-Boson Model. It has been extensively studied over the past thirty years by several varying techniques - ranging from the Feynman-Vernon influence-functional formulation [Fey65] to Liouville operator and projection methods [Fic90] and finally to exact mathematical results [Bac95].

Its popularity stems from the fact that it is the most simple non-trivial dissipative quantum system, consisting only of a two-state system and a bosonic bath that are linearly coupled in order to preserve the reflection symmetry of the system. Nevertheless, applications for the model are found in all fields of physics, starting from quantum optics and solid state physics to nuclear physics and chemistry.

In addition, from a mathematical and theoretical point of view, it attracts a lot of interest since it exhibits a Kosterlitz-Thouless transition for Ohmic coupling at $T = 0$ and a crossover from coherent to incoherent tunneling at finite temperature for all coupling types. Moreover it is related to many other prominent models in theoretical physics - most strikingly to the anisotropic Kondo Model.

The Kondo model has an even longer history. Initial results were obtained by Anderson by introducing his “poor man’s scaling” approach [And70] and by Anderson and Yuval by mapping the model onto the one-dimensional inverse square Ising Model [And71]. For the latter model Dyson proved the existence of a phase transition [Dys69].

The Kondo Model as well as the Spin-Boson Model belong to the so called strong-coupling problems which make the use of renormalization group techniques almost indispensable. The Kondo Model was first “solved” by Wilson employing the numerical renormalization group [Wil75]. These ideas were also applied to the Spin-Boson Model [Cos96].

Interest in dissipative *quantum* systems came up with tunnel experiments in Josephson junctions. At low temperatures the phase difference between the two superconducting devices has to be treated as a quantum mechanical degree of freedom that moves in a periodic potential. Since the potential shows two degenerate minima, one can project the system onto the two lowest lying non-interacting energy states which are coupled by the tunnel matrix element Δ.

Caldeira and Leggett pointed out that the interaction of the quantum mechanical degree of freedom with the environment has to be taken into account in order to account for the observed experimental data, i.e. strong suppression or destruction of quantum mechanical coherence. Furthermore, they illustrated that the environment can be modeled by a set of harmonic oscillators [Cal83].

In 1987 Leggett, Chakravarty, Dorsey, Fisher, Grag and Zwerger [Leg87] summarized the theoretical efforts on the Spin-Boson Model in Ref. [Leg87], propagating the Non-Interacting Blip Approximation (NIBA). This method is based on the Feynman-Vernon influence-functional approach and formulates the problem as one single path integral over four different states, two diagonal states and two off-diagonal states. Therefore, it makes explicit use of the simple structure of the two-level system. Decoupling the path integral by assuming that the "time" spent in the two off-diagonal states is short compared to the "time" spent in the two diagonal states corresponds to a perturbative treatment in the tunnel-matrix element Δ and yields analytic results for time dependent correlation functions at $T = 0$.

For Ohmic coupling the NIBA is justified for $\Delta/\omega_c \ll 1$ at the Toulouse point [Tou70] and for large and small coupling constants, and thus covers a wide range of the parameter space. It yields good results for the spectral function in the short- and intermediate time regime. Nevertheless it fails to predict the correct long-time behaviour.

This failure can be roughly understood by noting that the Feynman-Vernon influence-functional approach is based on the Lagrangian formulation of the system. Approximations within this formalism may lead to imaginary eigenvalues of the corresponding Hamiltonian and thus predict exponential decay of all time-dependent correlation functions. Since the NIBA takes all powers of Δ into consideration it yields an *algebraic* decay but nevertheless with a wrong non-universal exponent.

Evidently the Flow Equation approach does not face this problem as even within approximations the Hamiltonian formulation of the system is preserved. Kehrein and Mielke were therefore able to calculate the spectral function via numerical integration of the Flow Equations which remains valid over all time scales for super-Ohmic, and, providing a small coupling constant, also for Ohmic coupling [Keh97]. This clearly demonstrates the non-perturbative renormalization approach of the Flow Equations. To check their results they employed the generalized Shiba relation which relates the static susceptibility to the dynamic susceptibility at zero energy.

The numerical solution of Kehrein and Mielke which is based on the analogy of the Flow Equations of the Spin-Boson Model and the Dissipative Harmonic Oscillator, breaks down for Ohmic baths at moderate to strong coupling constants and for the sub-Ohmic bath at all coupling strengths. Moreover, Kehrein and Mielke did not consider the model with finite bias, i.e. with broken reflection symmetry. This is motivation enough to try to extend the numerical solution to make predictions in the parameter regime not accessible by prior approaches.

4.1. The Model

Since the method we want to use is based on the Hamiltonian formulation we will adopt the well-established standpoint to describe both, system and bath, as an isolated system. Dissipation enters through the fact that once energy has been transferred from the system to the infinite bath it will take an infinite amount of time until it will be transferred back to the system and has thus dissipated. A general dissipative quantum system is thus often described by the following Hamiltonian, see [Cal83]:

$$H = \frac{\hat{p}^2}{2m} + V(\hat{q}) + \sum_\alpha \frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{1}{2}m_\alpha\omega_\alpha^2(\hat{x}_\alpha - \frac{c_\alpha}{m_\alpha\omega_\alpha}\hat{q})^2 \tag{4.1}$$

The operators are denoted by a hat which shall be dropped from now on. They obey the canonical commutation relations which read

$$[q,p] = i \quad , \quad [x_\alpha, p_{\alpha'}] = i\delta_{\alpha,\alpha'} \quad . \tag{4.2}$$

In order to describe dissipation we will be guided by the correspondence principal. The classical equation of dissipative motion reads $m\partial_t^2 q + \eta\partial_t q + \partial_q V(q) = 0$ with the phenomenological friction parameter η. The quantum mechanical coupling constants c_α can now be deduced from the path integral formulation such that the corresponding Lagrange equation for the particle yield the damping force $-\eta\partial_t q$. One then observes that the coupling constants only enter in the combination of the spectral function $J(\omega) \equiv \pi/2\sum_\alpha c_\alpha^2/(m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha)$. In the case of a constant friction parameter η one speaks of Ohmic coupling and the spectral function takes on the simple form $J(\omega) = \eta\omega$ for small ω.

Given that the potential $V(q)$ exhibits two spatially separated, degenerate minima and the excited states are energetically much higher than the highest energy scale of the system[1] we can truncate the Hilbert space of the one-particle Hamiltonian onto the Hilbert space of a two-level system, i.e. $p^2/(2m) + V(q) \to -\Delta\sigma_x/2$, where Δ denotes the tunnel-matrix element which couples the degenerate states. In second quantization the Hamiltonian thus reads

$$H = -\frac{\Delta}{2}\sigma_x + \sum_\alpha \omega_\alpha b_\alpha^\dagger b_\alpha + \frac{\sigma_z}{2}\sum_\alpha \lambda_\alpha(b_\alpha + b_\alpha^\dagger) + E_0 \quad , \tag{4.3}$$

where we used $q = -q_0\sigma_z/2$ and $\lambda_\alpha = q_0 c_\alpha/(2m_\alpha\omega_\alpha)^{1/2}$.

The operators $b_\alpha^{(\dagger)}$ resemble the bath degrees of freedom and σ_i with $i = x, y, z$ denote the Pauli spin matrices. They obey the canonical commutation relations and the spin-1/2 algebra respectively. The constant energy shift is usually given by $E_0 = q_0^2/4\sum_\alpha \lambda_\alpha^2/\omega_\alpha$. The energy shift E_0 must be finite in order that the Hamiltonian is bounded from below. This yields a restriction on the coupling constants λ_α.

[1] Since we are generally dealing with $T = 0$ this energy scale is given by the cutoff frequency of the bosonic bath, i.e. ω_c.

The Hamiltonian (4.3) resembles an effective Hamiltonian where the high energy degrees of freedom of the bath were already integrated out down to the bath cutoff ω_c by employing the Born-Oppenheimer approximation. The tunnel-matrix element Δ thus depends on this arbitrary energy scale and all physical results must be independent of the cutoff ω_c. For Ohmic coupling one obtains $\Delta \propto (\omega_c)^\alpha$ with the dimensionless coupling constant $\alpha \equiv \eta q_0^2/(2\pi)$ and the only combination of Δ and ω_c that yields the units of an energy and is independent of ω_c is thus given by $\Delta_{\text{eff}} \propto \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$. All physical observables should only depend on this effective tunnel-matrix element. The expression for Δ_{eff} already alludes to the localization phenomena at $\alpha_c = 1$, first observed by Chakravarty [Cha82] and Bray and Moore [Bra82].

In Eq. (4.3) we included the constant q_0 which resembles the distance between the two minima. The natural extention of the Spin-Boson Model will include more than two minima and is discussed in Chapter 5. In the following we set $q_0 = 1$.

4.2. Non-Universal Asymptotic Behaviour

In this section we will first recall the solution of Kehrein and Mielke and also present a slightly different version to their approach. The Flow Equations will then be numerically integrated, choosing a realization which exhibits non-universal asymptotic behaviour. Since then the asymptotic spectral function will be centered around the renormalized tunnel-matrix element, Kehrein and Mielke were able to map the asymptotic Flow Equations of the Spin-Boson Model onto the asymptotic Flow Equations of the Dissipative Harmonic Oscillator. One thus can employ the exact solution of the Dissipative Harmonic Oscillator outlined in Section 2.3.

4.2.1. Standard Generator

We will briefly recall the approach of Kehrein and Mielke, outlined in Ref. [Keh97]. The generator η of the infinitesimal unitary transformations is chosen to be

$$\begin{aligned}\eta &= i\sigma_y \sum_\alpha \eta^y_\alpha (b_\alpha + b^\dagger_\alpha) + \sigma_z \sum_\alpha \eta^z_\alpha (b_\alpha - b^\dagger_\alpha) + \sum_{\alpha,\alpha'} \eta^e_{\alpha,\alpha'} (b_\alpha + b^\dagger_\alpha)(b_{\alpha'} - b^\dagger_{\alpha'}) \\ &\equiv \eta^{y,1} + \eta^{z,1} + \eta^{e,2} \quad .\end{aligned} \tag{4.4}$$

The commutator $[\eta, H]$ yields the following contributions:

$$[\eta^{y,1}, H] = -\Delta\sigma_z \sum_\alpha \eta^y_\alpha (b_\alpha + b^\dagger_\alpha) + i\sigma_y \sum_\alpha \eta^y_\alpha \omega_\alpha (b_\alpha - b^\dagger_\alpha) - \sigma_x \sum_{\alpha,\alpha'} \eta^y_\alpha \lambda_{\alpha'} (b_\alpha + b^\dagger_\alpha)(b_{\alpha'} + b^\dagger_{\alpha'}) \tag{4.5}$$

$$[\eta^{z,1}, H] = -i\sigma_y \Delta \sum_\alpha \eta^z_\alpha (b_\alpha - b^\dagger_\alpha) + \sigma_z \sum_\alpha \eta^z_\alpha \omega_\alpha (b_\alpha + b^\dagger_\alpha) + \sum_\alpha \eta^z_\alpha \lambda_\alpha \tag{4.6}$$

$$[\eta^{e,2}, H] = \sum_{\alpha,\alpha'} \eta^e_{\alpha,\alpha'} \omega_\alpha (b_\alpha - b^\dagger_\alpha)(b_{\alpha'} - b_{\alpha'}) + \sum_{\alpha,\alpha'} \eta^e_{\alpha,\alpha'} \omega_{\alpha'} (b_\alpha + b^\dagger_\alpha)(b_{\alpha'} + b^\dagger_{\alpha'}) + \sigma_z \sum_{\alpha,\alpha'} \eta^e_{\alpha,\alpha'} \lambda_{\alpha'} (b_\alpha + b^\dagger_\alpha) \tag{4.7}$$

For the Hamiltonian to remain form-invariant, normal ordered bosonic bilinears are neglected and the constants of the generator have to satisfy the following relations:

$$\eta^z_\alpha \Delta - \eta^y_\alpha \omega_\alpha = 0 \tag{4.8}$$

$$\eta^e_{\alpha,\alpha'} \omega_\alpha + \eta^e_{\alpha',\alpha} \omega_{\alpha'} = 0 \tag{4.9}$$

$$\eta^e_{\alpha,\alpha'} \omega_{\alpha'} + \eta^e_{\alpha',\alpha} \omega_\alpha - (\eta^y_\alpha \lambda_{\alpha'} + \eta^y_{\alpha'} \lambda_\alpha)\langle\sigma_x\rangle = 0 \tag{4.10}$$

With $\partial_\ell H = [\eta, H]$ this yields the following Flow Equations

$$\partial_\ell \Delta = 2\sum_\alpha \eta^y_\alpha \lambda_\alpha (1 + 2n_\alpha) \quad , \quad \partial_\ell E_0 = \sum_\alpha \eta^z_\alpha \lambda_\alpha$$
$$\partial_\ell \lambda_\alpha = 2(\eta^z_\alpha \omega_\alpha - \Delta \eta^y_\alpha + \sum_{\alpha'} \eta^e_{\alpha,\alpha'} \lambda_{\alpha'}) \tag{4.11}$$

We have neglected the flow of the bosonic modes ω_α which vanishes as $1/N$, N being the number of modes. Further, we introduced the Bose function $n_\alpha \equiv= (e^{\beta\omega_\alpha} - 1)^{-1}$ that stems from the normal ordering procedure.

One can determine the constants of the generator from the homogeneous equations (4.8) - (4.10) up to a function $f(\omega_\alpha, \ell)$. One finds $\eta^y_\alpha = \Delta\lambda_\alpha f(\omega_\alpha, \ell)/2$, $\eta^z_\alpha = \omega_\alpha \lambda_\alpha f(\omega_\alpha, \ell)/2$, $\eta^e_{\alpha,\alpha'} = -\Delta\langle\sigma_x\rangle\lambda_\alpha\lambda_{\alpha'}\omega_{\alpha'}/(\omega^2_\alpha - \omega^2_{\alpha'})(f(\omega_\alpha, \ell) + f(\omega_{\alpha'}, \ell))/2$ and thus obtains with the spectral function

$$J(\omega) = \sum_\alpha \lambda^2_\alpha \delta(\omega - \omega_\alpha) \tag{4.12}$$

the following coupled integro-differential equations:

$$
\begin{aligned}
\partial_\ell \Delta &= \Delta \int d\omega J(\omega,\ell) f(\omega,\ell)(1+2n(\omega)) \\
\partial_\ell E_0 &= \int d\omega J(\omega,\ell)\omega f(\omega,\ell)/2 \\
\partial_\ell J(\omega,\ell) &= 2J(\omega,\ell)(\omega^2-\Delta^2) f(\omega,\ell) \\
&\quad - 2\Delta\langle\sigma_x\rangle J(\omega,\ell)\int d\omega' \frac{J(\omega',\ell)\omega'}{\omega^2-\omega'^2}(f(\omega,\ell)+f(\omega',\ell))
\end{aligned}
\tag{4.13}
$$

To determine correlation functions the observables have to be transformed by the same sequence of unitary transformations as the Hamiltonian. Kehrein and Mielke made the following ansatz:

$$
\sigma_z(\ell) = h(\ell)\sigma_z + \sigma_x \sum_\alpha \chi_\alpha(\ell)(b_\alpha + b_\alpha^\dagger) \tag{4.14}
$$

The Flow Equations $\partial_\ell \sigma_z = [\eta, \sigma_z]$ do not close and normal ordered bosonic bilinears are neglected. One then obtains:

$$
\begin{aligned}
\partial_\ell h &= 2\sum_\alpha \eta_\alpha^y \chi_\alpha (2n_\alpha + 1) = \Delta \sum_\alpha \lambda_\alpha \chi_\alpha f(\omega_\alpha,\ell) \\
\partial_\ell \chi_\alpha &= -2h\eta_\alpha^y + 2\sum_{\alpha'} \eta_{\alpha,\alpha'}^e \chi_{\alpha'} \\
&= -h\Delta\lambda_\alpha f(\omega_\alpha,\ell) - \Delta\langle\sigma_x\rangle\lambda_\alpha \sum_{\alpha'} \frac{\lambda_{\alpha'}\chi_{\alpha'}\omega_{\alpha'}}{\omega_\alpha^2-\omega_{\alpha'}^2}(f(\omega_\alpha,\ell)+f(\omega_{\alpha'},\ell))
\end{aligned}
\tag{4.15}
$$

Let us look forward for a moment. In Chapter 5 we will compare these Flow Equations with Flow Equations obtained from a periodic model. In order to identify these we will have to neglect two-boson processes, i.e. contributions that stem from the generator $\eta^{e,2}$. For the comparison it is also useful to introduce the spectral function $S(\omega) = \sum_\alpha \lambda_\alpha \chi_\alpha \delta(\omega - \omega_\alpha)$. Thus neglecting the two-boson processes we obtain the following set of Flow Equations to be compared with in Chapter 5:

$$
\begin{aligned}
\partial_\ell h &= \Delta \int d\omega S(\omega,\ell) f(\omega,\ell) \\
\partial_\ell S(\omega,\ell) &= -\Delta h J(\omega,\ell) + S(\omega,\ell)(\omega^2-\Delta^2)
\end{aligned}
\tag{4.16}
$$

Let us return to the Spin-Boson Model and focus on the dynamical properties. These can be described by the symmetrized equilibrium correlation function $C(t)$ defined as

$$
C(t) = \langle e^{iH_\infty t}\sigma_z(\ell=\infty)e^{-iH_\infty t}\sigma_z(\ell=\infty) + (t\to -t)\rangle/2 \quad , \tag{4.17}
$$

where the canonical average is taken over the fixed point Hamiltonian $H_\infty \equiv H(\ell = \infty)$. The time evolution becomes trivial for $\ell \to \infty$ and inserting the fixed point values of the parameters of the Hamiltonian and the observable we obtain

$$C(t) = h^2(\ell = \infty)\cos(\Delta_\infty t) + \sum_\alpha \chi_\alpha^2(\ell = \infty)(2n_\alpha + 1)\cos(\omega_\alpha t) \quad . \tag{4.18}$$

Following the same argumentation as in the case of the Dissipative Harmonic Oscillator we conclude that $h(\ell = \infty) = 0$. The one-sided Fourier transform at $T = 0$ is then given by

$$C(\omega) = \sum_\alpha \chi_\alpha^2(\ell = \infty)\delta(\omega - \omega_\alpha) \quad . \tag{4.19}$$

4.2.2. Modified Generator

We will now present a slightly different version of the previous Flow Equations and treat the flow of operators which are bilinear in the bosonic operators $b_\alpha^{(\dagger)}$ exactly. To accomplish this, the generator η of the infinitesimal unitary transformations is now chosen to be

$$\begin{aligned}\eta &= i\sigma_y \sum_\alpha \eta_\alpha^y (b_\alpha + b_\alpha^\dagger) + \sigma_z \sum_\alpha \eta_\alpha^z (b_\alpha - b_\alpha^\dagger) + \sigma_x \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}^x (b_\alpha + b_\alpha^\dagger)(b_{\alpha'} - b_{\alpha'}^\dagger) \\ &\equiv \eta^{y,1} + \eta^{z,1} + \eta^{x,2} \quad .\end{aligned} \tag{4.20}$$

For η to be anti-hermitian, $\eta_{\alpha,\alpha}^x = 0$ must hold.

The commutator $[\eta, H]$ differs from Eqs. (4.5) - (4.7) only in the following contribution:

$$\begin{aligned}[\eta^{x,2}, H] &= \sigma_x \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}^x \omega_\alpha (b_\alpha - b_\alpha^\dagger)(b_{\alpha'} - b_{\alpha'}) + \sigma_x \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}^x \omega_{\alpha'} (b_\alpha + b_\alpha^\dagger)(b_{\alpha'} + b_{\alpha'}^\dagger) \\ &- \frac{1}{2} i\sigma_y \sum_{\alpha,\alpha',\alpha''} \eta_{\alpha,\alpha'}^x \lambda_{\alpha''} \{(b_\alpha + b_\alpha^\dagger)(b_{\alpha'} - b_{\alpha'}^\dagger), (b_{\alpha''} + b_{\alpha''}^\dagger)\}\end{aligned} \tag{4.21}$$

The anti-commutator yields $\{x_\alpha p_{\alpha'}, x_{\alpha''}\} = 2 : x_\alpha x_{\alpha''} p_{\alpha'} : + 2\delta_{\alpha,\alpha''} p_{\alpha'}(1 + 2n_\alpha)$, where we defined $x_\alpha \equiv (b_\alpha + b_\alpha^\dagger)$, $p_\alpha \equiv (b_\alpha - b_\alpha^\dagger)$. For the Hamiltonian to remain form-invariant, normal ordered bosonic *trilinear* are neglected and the constants of the generator have to satisfy the following relations:

$$\eta_\alpha^z \Delta - \eta_\alpha^y \omega_\alpha + \textstyle\sum_{\alpha'} \eta_{\alpha',\alpha}^x \lambda_{\alpha'}(1 + 2n_{\alpha'}) = 0 \tag{4.22}$$

$$\eta_{\alpha,\alpha'}^x \omega_\alpha + \eta_{\alpha',\alpha}^x \omega_{\alpha'} = 0 \tag{4.23}$$

$$\eta_{\alpha,\alpha'}^x \omega_{\alpha'} + \eta_{\alpha',\alpha}^x \omega_\alpha - (\eta_\alpha^y \lambda_{\alpha'} + \eta_{\alpha'}^y \lambda_\alpha) = 0 \tag{4.24}$$

Further, we first normal order the operators which shall vanish. With $\partial_\ell H = [\eta, H]$ this yields the following Flow Equations:

$$\partial_\ell \Delta = 2\sum_\alpha \eta_\alpha^y \lambda_\alpha (2n_\alpha + 1) \quad , \quad \partial_\ell E_0 = \sum_\alpha \eta_\alpha^z \lambda_\alpha \quad , \quad \partial_\ell \lambda_\alpha = 2\eta_\alpha^z \omega_\alpha - 2\Delta \eta_\alpha^y \tag{4.25}$$

From the homogeneous equations (4.22) - (4.24) the constants of the generator are determined up to a function $f(\omega_\alpha,\ell)$. One finds $\eta^y_\alpha = \Delta\lambda_\alpha f(\omega_\alpha,\ell)/2$, $\eta^z_\alpha = \omega_\alpha\lambda_\alpha f(\omega_\alpha,\ell)/2 + \sum_{\alpha'}\lambda_\alpha\lambda^2_{\alpha'}\omega_\alpha/(\omega^2_\alpha - \omega^2_{\alpha'})(f(\omega_\alpha,\ell) + f(\omega_{\alpha'},\ell))/2$, $\eta^x_{\alpha,\alpha'} = -\Delta\lambda_\alpha\lambda_{\alpha'}\omega_{\alpha'}/(\omega^2_\alpha-\omega^2_{\alpha'})(f(\omega_\alpha,\ell)+f(\omega_{\alpha'},\ell))/2$ and thus obtains with the spectral function

$$J(\omega) = \sum_\alpha \lambda^2_\alpha \delta(\omega - \omega_\alpha) \tag{4.26}$$

the following coupled integro-differential equations:

$$\partial_\ell \Delta = \Delta \int d\omega J(\omega,\ell) f(\omega,\ell)(2n(\omega)+1) \tag{4.27}$$

$$\begin{aligned}\partial_\ell E_0 = &\int d\omega J(\omega,\ell)\omega f(\omega,\ell)/2 \\ &+ \int d\omega J(\omega,\ell)\omega^2 \int d\omega' \frac{J(\omega',\ell)}{\omega^2-\omega'^2}(f(\omega,\ell)+f(\omega',\ell))/2\end{aligned} \tag{4.28}$$

$$\begin{aligned}\partial_\ell J(\omega,\ell) = &\, 2J(\omega,\ell)(\omega^2-\Delta^2) f(\omega,\ell) \\ &+ 2J(\omega,\ell)\omega^2 \int d\omega' \frac{J(\omega',\ell)}{\omega^2-\omega'^2}(f(\omega,\ell)+f(\omega',\ell))\end{aligned} \tag{4.29}$$

Notice that there is a sign change in front of the term of the two-boson processes relative to the Flow Equations of the previous subsection.

To determine correlation functions we again have to transform the observable. We make the following ansatz:

$$\sigma_z(\ell) = h(\ell)\sigma_z + \sum_\alpha \chi^e_\alpha(\ell)(b_\alpha + b^\dagger_\alpha) + \sigma_x \sum_\alpha \chi^x_\alpha(\ell)(b_\alpha + b^\dagger_\alpha) \tag{4.30}$$

The Flow Equations do not close and we will neglect normal ordered bosonic bilinears. One then obtains:

$$\begin{aligned}&\partial_\ell h = 2\sum_\alpha(\eta^y_\alpha\chi^x_\alpha(2n_\alpha+1) + \eta^z_\alpha\chi^e_\alpha) \\ &\partial_\ell\chi^e_\alpha = 2\sum_{\alpha'}\eta^x_{\alpha,\alpha'} \quad , \quad \partial_\ell\chi^x_\alpha = -2h\eta^y_\alpha + 2\sum_{\alpha'}\eta^x_{\alpha,\alpha'}\chi^e_{\alpha'}\chi^x_{\alpha'}\end{aligned} \tag{4.31}$$

Following the same lines as in the previous subsection we obtain for the one-sided Fourier transform of the symmetrized correlation function $C(t)$, defined in Eq. (4.17), the following expression:

$$C(\omega) = \sum_\alpha(\chi^e_\alpha(\ell=\infty) + \chi^x_\alpha(\ell=\infty))^2\delta(\omega-\omega_\alpha) \quad . \tag{4.32}$$

We want to remark that the Flow Equations of Eqs. (4.31) reduce to the Flow Equations of Eqs. (4.15) for $\ell\to\infty$ by replacing $\chi^x_\alpha + \chi^e_\alpha \to \chi_\alpha$, provided that we choose

$f(\omega_\alpha, \ell)$ such that the spectral function $J(\omega, \ell)$ is strongly peaked around $\omega = \Delta(\ell)$ for $\ell \to \infty$.[2] This observation will be useful because we will be able to use the same asymptotic analogy between the Spin-Boson Model and Dissipative Harmonic Oscillator which was pointed out by Kehrein and Mielke in the case of the standard generator.

4.2.3. Numerical Results

We will now determine time-dependent correlation functions by numerically solving the Flow Equations of the previous two subsections. The results are compared with the correlation functions obtained from the NIBA. We will further restrain ourselves to the case of Ohmic coupling and to $T = 0$.

We briefly summerize the results of the NIBA, outlined in Ref. [Leg87]. Within this approximation the correlation functions $P^{NI}(t) \equiv \langle \sigma_z(t) \rangle$ with $P^{NI}(t \leq 0) = 1$ and the symmetrized equilibrium correlation function $C^{NI}(t) \equiv \langle \sigma_z(t)\sigma_z + (t \to -t) \rangle/2$ yield the same expression. For $J(\omega) = 2\alpha\omega e^{-\omega/\omega_c}$ it is thus given by $C^{NI}(t) = E_{2(1-\alpha)}(-y^{2(1-\alpha)})$ with $y \equiv \Delta_{\text{eff}} t$ and

$$\Delta_{\text{eff}} \equiv (\cos(\pi\alpha)\Gamma(1-2\alpha))^{1/2(1-\alpha)} \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}. \tag{4.33}$$

Here $E_\nu(z) \equiv \sum_{k=0}^{\infty} z^k/\Gamma(\nu k + 1)$ denotes the Mittag-Leffler function [Gra85]. The series can be summed up using Hankel's contour integral representation for the reciprocal of the Γ function and evaluating the resultant integral by deformation of the contour. One obtains

$$C^{NI}(t) = \cos(\Delta_{\text{eff}} \cos(\frac{\pi}{2}\frac{\alpha}{1-\alpha})t) \exp(-(\Delta_{\text{eff}} \cos(\frac{\pi}{2}\frac{\alpha}{1-\alpha})t)) + C_{\text{inc}}^{NI}(t) \quad , \tag{4.34}$$

where the incoherent contribution is given by

$$C_{\text{inc}}^{NI}(y) = -\frac{\sin(2\pi\alpha)}{\pi} \int_0^\infty dz \frac{z^{2\alpha-1} e^{-zy}}{z^2 + 2z^{2\alpha}\cos(2\pi\alpha) + z^{4\alpha-2}} \quad . \tag{4.35}$$

From $C_{\text{inc}}^{NI}(y)$ and for $\alpha \neq 1/2$ the long-time behaviour of $C^{NI}(t)$ yields $C^{NI}(t) \to t^{-2(1-\alpha)}$, which is incorrect.[3]

In order to evaluate the symmetrized equilibrium function $C(t)$ by means of the Flow Equation technique reference to the exactly solvable Harmonic Oscillator proves

[2] This is our definition of non-universal asymptotic behaviour.

[3] The case $\alpha = 1/2$ yields exponential decay of $C(t)$ which is "even more" incorrect. A brief discussion on this singular point is given in the erratum of Ref. [Leg87].

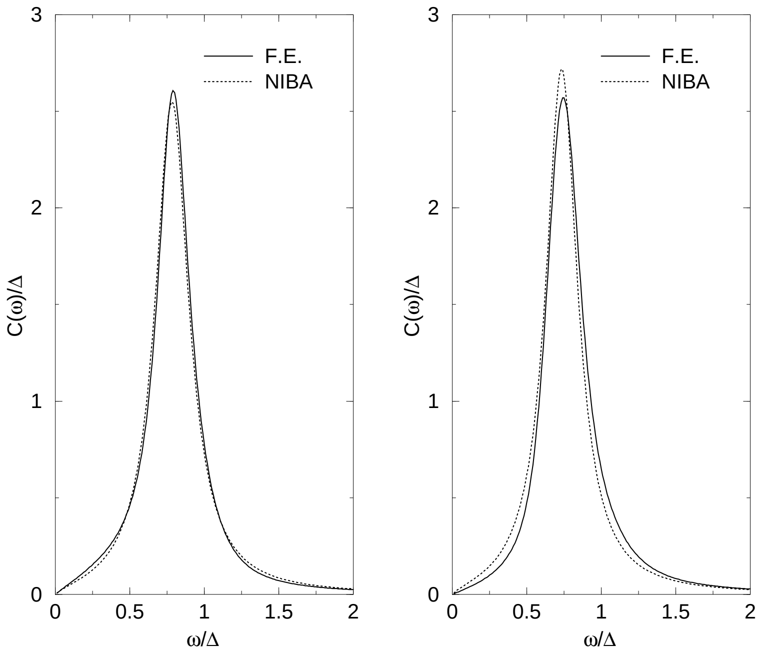

Figure 4.1.: The spectral function $C(\omega)$ obtained from the Flow Equation approach employing the standard generator (left hand side) and the modified generator (right hand side) for $J(\omega) = 2\alpha\omega\Theta(\omega_c - \omega)$ with $\alpha = 0.1$ and $\omega_c/\Delta = 10$, using the conservation law at $\Delta^2\ell^* = 10$. They are contrasted with $C^{NI}(\omega)$ for $\alpha = 0.1$ and suitable Δ_{eff}.

to be helpful. A detailed discussion is given in Ref. [Keh97]. Introducing the functions

$$S_2(z,\ell) = \sum_\alpha \frac{\chi_\alpha^2}{z-\omega_\alpha^2} \quad , \tag{4.36}$$

$$S_1(z,\ell) = \sum_\alpha \frac{\sqrt{\omega_\alpha\Delta}\chi_\alpha\lambda_\alpha}{z-\omega_\alpha^2} \quad , \tag{4.37}$$

$$S_0(z,\ell) = \sum_\alpha \frac{\omega_\alpha\lambda_\alpha^2}{z-\omega_\alpha^2} \quad , \tag{4.38}$$

one obtains the approximate relation

$$S_2(z,\ell=\infty) \approx S_2(z,\ell^*) - \frac{(h(\ell^*)+S_1(z,\ell^*))^2}{\Delta^2(\ell^*) - z + \Delta(\ell^*)S_0(z,\ell^*)} \quad . \tag{4.39}$$

The Flow Equations are now numerically integrated up to $\ell = \ell^*$ and $S_2(z,\ell=\infty)$ is then given by Eq. (4.39).[4] A check for the validity of the approximate relation is given by the invariance of $S_2(z,\ell=\infty)$ on ℓ^*.

[4]Remember the asymptotic replacement $\chi_\alpha^e + \chi_\alpha^x \rightarrow \chi_\alpha$ in the case of the modified generator, discussed in the end of subsection 4.2.2.

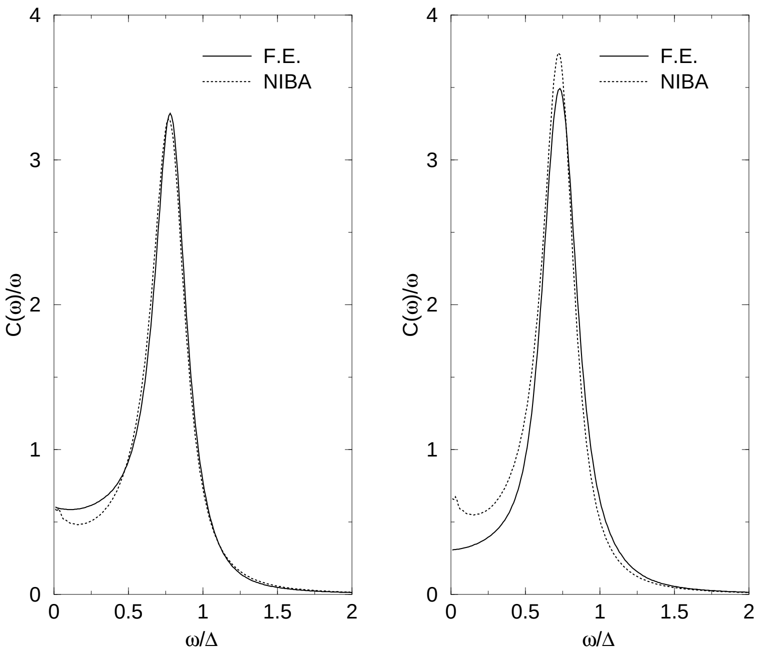

Figure 4.2.: The spectral function $C(\omega)/\omega$ obtained from the Flow Equation approach employing the standard generator (left hand side) and the modified generator (right hand side) for $J(\omega) = 2\alpha\omega\Theta(\omega_c - \omega)$ with $\alpha = 0.1$ and $\omega_c/\Delta = 10$, using the conservation law at $\Delta^2\ell^* = 10$. They are contrasted with $C^{NI}(\omega)/\omega$ for $\alpha = 0.1$ and suitable Δ_{eff}.

The one-sided Fourier transform $C(\omega) = \sum_\alpha \chi_\alpha^2(\ell = \infty)\delta(\omega - \omega_\alpha)$ of the correlation function $C(t) = \int_0^\infty d\omega C(\omega)\exp(i\omega t)$ is now obtained from $S_2(z, \ell = \infty)$ using $C(\omega) = 2\omega/\pi \text{Im} S_2(\omega^2 - i0, \ell = \infty)$. This implies an unusual normalization condition following from the initial condition $C^{NI}(t = 0) = 1$: $\int_0^\infty d\omega C^{NI}(\omega) = 1$. The corresponding quantity stemming from the NIBA is given by $C^{NI}(\omega) \propto \int_0^\infty dt C^{NI}(t)\cos(\omega t)$ with a suitable normalization constant.

For the numerical calculations the arbitrary function $f(\omega_\alpha, \ell)$ has to be specified. According to Kehrein and Mielke $f(\omega_\alpha, \ell)$ is chosen such that the spectral function $J(\omega, \ell)$ is monotonically decreasing if one neglects the non-linear term in the corresponding differential equation, i.e. $f(\omega, \ell) = -(\omega - \Delta(\ell))/(\omega + \Delta(\ell))$.

A very sensitive test for the numerical results is provided by the Shiba relation [Shi75] generalized to the the Spin-Boson Model in Ref. [Sas90]. A mathematically rigorous proof is found in Ref. [New99]. For an Ohmic bath this reads

$$\lim_{\omega \to 0} \frac{C(\omega)}{\omega} = 2\alpha(2\chi_0)^2 \quad , \tag{4.40}$$

with the static susceptibility $\chi_0 = \int_0^\infty C(\omega)/(2\omega)d\omega$. As was first pointed out in Ref.

[Keh97], the Flow Equations yield good agreement for small coupling strengths, i.e. $\alpha \leq 0.1$.

In Figure 4.1 the spectral function $C(\omega)$ obtained from integrating the Flow Equations up to $\ell^* = 10/\Delta^2$ and making use of the conservation law of Eq. (4.39) is compared with the NIBA. The left hand side shows the results for the standard generator and the right hand side the results for the modified generator. For both versions of the Flow Equations we chose an initial spectral function with $\alpha = 0.1$ and a sharp cutoff at $\omega_c = 10\Delta$. The parameters for the NIBA were chosen to be $\alpha = 0.1$ and Δ_{eff} such that the maxima of the two curves coincide.

One sees that both versions of the Flow Equations agree with the NIBA in the intermediate and short-time regime. In the long-time regime only the Flow Equation approach yields the correct behaviour, i.e. $C(\omega) \propto \omega$. This can be seen more explicitly in Figure 4.2 where $C(\omega)/\omega$ is plotted.

To contrast the results obtained from the two generators, again the Shiba relation proves to be useful. For the standard generator we obtain $\lim_{\omega\to 0} C(\omega)/\omega \approx 0.58$ and $2\alpha(2\chi_0)^2 \approx 0.41$ whereas for the modified generator the numerical calculations yield $\lim_{\omega\to 0} C(\omega)/\omega \approx 0.31$ and $2\alpha(2\chi_0)^2 \approx 0.39$. Notice that whereas the static susceptibility is approximately the same in both approaches, the limiting values of $C(\omega)/\omega$ for $\omega \to 0$ vary significantly. We obtain an improvement in the relative error in the case of the modified generator as could have been expected since in this approach one treats bilinear bosonic operators *exactly*.

4.3. General Flow Equations

In this section we want to address a more general model, i.e. we will include a finite bias ϵ in our considerations. It will turn out that the generator is then - up to a constant which sets the scale of the ℓ-flow - completely determined by demanding a form-invariant flow of the Hamiltonian. This generator will lead to universal asymptotic behaviour. By this we mean that the tunnel-matrix element Δ and the bias ϵ tend to zero for $\ell \to \infty$ so that no physical information is contained in the fixed point Hamiltonian $H(\ell = \infty)$.

The universal asymptotic behaviour is also a consequence if one formulates the Flow Equations for a unitarily equivalent Hamiltonian for which the reflection symmetry is broken even when no bias is applied. Since these calculations are similar to the ones that we are going to present here we have only added them in Appendix D.

In the first part of this section we will formulate the Flow Equations in a general manner. By setting up the truncation scheme we are guided by the conclusions of Chapter 3, i.e. we will define distinguished bosonic modes. Further a self-consistent determination of the one-particle expectation values is presented and it will be pointed out that this can qualitatively change the flow of the applied bias ϵ.

We will then formulate the Flow Equations of the observables up to second order in the bosonic bath operators $b_\alpha^{(\dagger)}$. Including the second order might lead to significant improvements according to the observations of the last chapter. Further we choose an ansatz for the observable flow that depends on the ℓ-dependent distinguished modes.

Since we are dealing with Flow Equations which exhibit an universal asymptotic behaviour, we will set up differential equations that determine the asymptotic coupling function and the asymptotic observable flow in the next subsection. It will turn out that these differential equations are almost identical to the differential equations that govern the asymptotic behaviour of the Dissipative Harmonic Oscillator discussed in subsection 2.3.2.

In the last part of this section we will present the numerical results of this approach. Since the fixed point Hamiltonian of the form-invariant flow contains no physical information the flow of the observable becomes crucial. We will be able to recover the results for the effective tunnel-matrix element of the NIBA, but we fail in completely describing the symmetrized equilibrium correlation function $C(\omega)$.

4.3.1. Flow Equations for the Hamiltonian

Applying a finite bias ϵ the Spin-Boson Hamiltonian is now given by

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_\alpha b_\alpha^\dagger b_\alpha + \sigma_z \frac{\lambda_\alpha}{2}(b_\alpha + b_\alpha^\dagger) + E \quad . \tag{4.41}$$

The operators $b_\alpha^{(\dagger)}$ resemble the bath degrees of freedom and σ_i with $i = x, y, z$ denote the Pauli spin matrices. They obey the canonical commutation relations and the spin-1/2 algebra respectively. Summation over the bath modes α is implied.

Generally new interaction terms are created during the flow. Therefore, we will consider the following extended Hamiltonian which takes all coupling terms into account that are linear in the bosonic ladder operators:

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_\alpha b_\alpha^\dagger b_\alpha + \sigma_i \frac{\lambda_\alpha^i}{2}(b_\alpha + b_\alpha^\dagger) + i\sigma_y \frac{\lambda_\alpha^y}{2}(b_\alpha - b_\alpha^\dagger) + E \tag{4.42}$$

Summation over $i = e, x, z$ with $\sigma_e \equiv 1$ is implied. The initial conditions for the coupling constants are given by $\lambda_\alpha^e = \lambda_\alpha^x = \lambda_\alpha^y = 0$ and $\lambda_\alpha^z = \lambda_\alpha$.

The Hamiltonian can formally be diagonalized in the following way:

$$\begin{aligned} H = &-\frac{\Delta'}{2}\sigma_x + \frac{\epsilon'}{2}\sigma_z + E' \\ &+ \omega_\alpha(b_\alpha^\dagger + \sigma_i\frac{\lambda_\alpha^i}{2\omega_\alpha} + i\sigma_y\frac{\lambda_\alpha^y}{2\omega_\alpha})(b_\alpha + \sigma_i\frac{\lambda_\alpha^i}{2\omega_\alpha} - i\sigma_y\frac{\lambda_\alpha^y}{2\omega_\alpha}) \quad , \end{aligned} \tag{4.43}$$

with $\Delta' \equiv \Delta + \frac{\lambda_\alpha^e\lambda_\alpha^x}{\omega_\alpha} - \frac{\lambda_\alpha^y\lambda_\alpha^z}{\omega_\alpha}$, $\epsilon' \equiv \epsilon - \frac{\lambda_\alpha^e\lambda_\alpha^z}{\omega_\alpha} - \frac{\lambda_\alpha^x\lambda_\alpha^y}{\omega_\alpha}$ and $E' \equiv E - \frac{\lambda_\alpha^i\lambda_\alpha^i}{4\omega_\alpha} - \frac{\lambda_\alpha^y\lambda_\alpha^y}{4\omega_\alpha}$.

Since $\langle i\sigma_y\rangle = 0$ the distinguished bosonic modes are resembled by $\bar{b}_\alpha \equiv b_\alpha + \langle\sigma_i\rangle\frac{\lambda^i_\alpha}{2\omega_\alpha}$. Rewritten in these modes the Hamiltonian of Eq. (4.42) reads

$$H = -\frac{\bar{\Delta}}{2}\sigma_x + \frac{\bar{\epsilon}}{2}\sigma_z + \bar{E} + \omega_\alpha \bar{b}^\dagger_\alpha \bar{b}_\alpha + \sigma_i \frac{\bar{\lambda}^i_\alpha}{2}(\bar{b}_\alpha + \bar{b}^\dagger_\alpha) + i\sigma_y \frac{\bar{\lambda}^y_\alpha}{2}(\bar{b}_\alpha - \bar{b}^\dagger_\alpha) \quad , \tag{4.44}$$

where we introduced the renormalized parameters

$$\bar{\Delta} \equiv \Delta + \langle\sigma_i\rangle \frac{\lambda^i_\alpha \lambda^x_\alpha}{\omega_\alpha} \quad , \quad \bar{\epsilon} \equiv \epsilon - \langle\sigma_i\rangle \frac{\lambda^i_\alpha \lambda^z_\alpha}{\omega_\alpha} \quad , \tag{4.45}$$

$$\bar{E} \equiv E - \langle\sigma_i\rangle \frac{\lambda^i_\alpha \lambda^e_\alpha}{2\omega_\alpha} - \langle\sigma_i\rangle\langle\sigma_{i'}\rangle \frac{\lambda^i_\alpha \lambda^{i'}_\alpha}{4\omega_\alpha} \quad , \tag{4.46}$$

$$\bar{\lambda}^e_\alpha \equiv \lambda^e_\alpha - \langle\sigma_i\rangle\lambda^i_\alpha \quad , \quad \bar{\lambda}^x_\alpha \equiv \lambda^x_\alpha \quad , \quad \bar{\lambda}^y_\alpha \equiv \lambda^y_\alpha \quad , \quad \bar{\lambda}^z_\alpha \equiv \lambda^z_\alpha \quad . \tag{4.47}$$

Considering the two dimensional Hamiltonian this yields a set of self-consistent equations:

$$\langle\sigma_x\rangle = \bar{\Delta}/\bar{R} \quad , \quad \langle\sigma_z\rangle = -\bar{\epsilon}/\bar{R} \quad , \quad \text{with } \bar{R}^2 \equiv \bar{\Delta}^2 + \bar{\epsilon}^2. \tag{4.48}$$

The expectation values of the one-particle Hamiltonian can thus be determined within a mean-field approximation.

To set up the Flow Equations for the parameters of the Hamiltonian, we go back to the representation of H given in Eq. (4.42). The anti-hermitian generator for the infinitesimal unitary transformations η shall be given by

$$\begin{aligned} \eta &= i\sigma_y\eta^y + \sigma_i\eta^i_\alpha(b_\alpha - b^\dagger_\alpha) + i\sigma_y\eta^y_\alpha(b_\alpha + b^\dagger_\alpha) + \eta^e_{\alpha,\alpha'}(b_\alpha + b^\dagger_\alpha)(b_{\alpha'} - b^\dagger_{\alpha'}) \\ &\equiv \eta^{y,0} + \sum_i \eta^{i,1} + \eta^{y,1} + \eta^{e,2} \quad . \end{aligned} \tag{4.49}$$

To be more general we could also have included terms which are bilinear in the bosonic operators and coupled to the three Pauli spin matrices, i.e. $\eta^{i,2} \equiv \sigma_i\eta^i_{\alpha,\alpha'}(b_\alpha + b^\dagger_\alpha)(b_{\alpha'} - b^\dagger_{\alpha'})$ and $\eta^{y,\pm,2} \equiv \sigma_i\eta^{y,\pm}_{\alpha,\alpha'}(b_\alpha \pm b^\dagger_\alpha)(b_{\alpha'} \pm b^\dagger_{\alpha'})$. This was the difference between the standard and the modified generator of the last section. Here we only want to sketch the general picture. Extentions are straightforward.

To obtain the Flow Equations $\partial_\ell H = [\eta, H]$ we have to evaluate the commutator

$[\eta, H]$:

$$
\begin{aligned}
[\eta^{y,0}, H] &= -\sigma_z \Delta \eta^y - \sigma_x \epsilon \eta^y + \sigma_z \eta^y \lambda^x_\alpha x_\alpha - \sigma_x \eta^y \lambda^z_\alpha x_\alpha && (4.50)\\
[\eta^{e,1}, H] &= \eta^e_\alpha \omega_\alpha x_\alpha + \eta^e_\alpha \lambda^e_\alpha + \sigma_x \eta^e_\alpha \lambda^x_\alpha + \sigma_z \eta^e_\alpha \lambda^z_\alpha && (4.51)\\
[\eta^{x,1}, H] &= -i\sigma_y \epsilon \eta^x_\alpha p_\alpha + \sigma_x \eta^x_\alpha \omega_\alpha x_\alpha + \eta^x_\alpha \lambda^x_\alpha - \sigma_z \eta^x_\alpha \lambda^y_{\alpha'} p_\alpha p_{\alpha'}\\
&\quad - i\sigma_y \eta^x_\alpha \frac{\lambda^z_{\alpha'}}{2}\{p_\alpha, x_{\alpha'}\} && (4.52)\\
[\eta^{y,1}, H] &= -\sigma_z \Delta \eta^y_\alpha x_\alpha - \sigma_x \epsilon \eta^y_\alpha x_\alpha + i\sigma_y \eta^y_\alpha \omega_\alpha p_\alpha + \sigma_z \eta^y_\alpha \lambda^x_{\alpha'} x_\alpha x_{\alpha'}\\
&\quad + \eta^y_\alpha \lambda^y_\alpha - \sigma_x \eta^y_\alpha \lambda^z_{\alpha'} x_\alpha x_{\alpha'} && (4.53)\\
[\eta^{z,1}, H] &= -i\sigma_y \Delta \eta^z_\alpha p_\alpha + \sigma_z \eta^z_\alpha \omega_\alpha x_\alpha + i\sigma_y \eta^z_\alpha \frac{\lambda^x_{\alpha'}}{2}\{p_\alpha, x_{\alpha'}\}\\
&\quad + \sigma_x \eta^z_\alpha \lambda^y_{\alpha'} p_\alpha p_{\alpha'} + \eta^z_\alpha \lambda^z_\alpha && (4.54)\\
[\eta^{e,2}, H] &= \eta^e_{\alpha,\alpha'} \omega_\alpha p_\alpha p_{\alpha'} + \eta^e_{\alpha,\alpha'} \omega_{\alpha'} x_\alpha x_{\alpha'} + \sigma_i \eta^e_{\alpha,\alpha'} \lambda^i_{\alpha'} x_\alpha - i\sigma_y \eta^e_{\alpha',\alpha} \lambda^y_{\alpha'} p_\alpha && (4.55)
\end{aligned}
$$

For brevity we introduced $x_\alpha \equiv (b_\alpha + b^\dagger_\alpha)$ and $p_\alpha \equiv (b_\alpha - b^\dagger_\alpha)$.

In order to close the Flow Equations based on the Hamiltonian (4.42) we will neglect normal ordered bosonic bilinears:

$$
\begin{aligned}
\mathcal{O}_1 &= -\sigma_x \eta^y_\alpha \lambda^z_{\alpha'} :\bar{x}_\alpha \bar{x}_{\alpha'}: \quad , \quad \mathcal{O}_2 = \sigma_z \eta^y_\alpha \lambda^x_{\alpha'} :\bar{x}_\alpha \bar{x}_{\alpha'}: \quad , && (4.56)\\
\mathcal{O}_3 &= \sigma_x \eta^z_\alpha \lambda^y_{\alpha'} :\bar{p}_\alpha \bar{p}_{\alpha'}: \quad , \quad \mathcal{O}_4 = -\sigma_z \eta^x_\alpha \lambda^y_{\alpha'} :\bar{p}_\alpha \bar{p}_{\alpha'}: \quad , && (4.57)\\
\mathcal{O}_5 &= i\sigma_y (\eta^z_\alpha \frac{\lambda^x_{\alpha'}}{2} - \eta^x_\alpha \frac{\lambda^z_{\alpha'}}{2}) :\{\bar{p}_\alpha, \bar{x}_{\alpha'}\}: \quad , && (4.58)\\
\mathcal{O}_6 &= \eta^e_{\alpha,\alpha'} \omega_\alpha :\bar{p}_\alpha \bar{p}_{\alpha'}: \quad , \quad \mathcal{O}_7 = \eta^e_{\alpha,\alpha'} \omega_{\alpha'} :\bar{x}_\alpha \bar{x}_{\alpha'}: \quad . && (4.59)
\end{aligned}
$$

Notice that we normal order with respect to the shifted bosonic modes $\bar{x}_\alpha \equiv (\bar{b}_\alpha + \bar{b}^\dagger_\alpha)$ and $\bar{p}_\alpha \equiv (\bar{b}_\alpha - \bar{b}^\dagger_\alpha) = p_\alpha$. This truncation scheme is motivated by the results of Chapter 3 and Appendix D. It leads to the following Flow Equations:[5]

$$
\begin{aligned}
\partial_\ell \Delta &= 2\epsilon\eta^y - 2\eta^e_\alpha \lambda^x_\alpha + 2\eta^z_\alpha \lambda^y_\alpha 1_\alpha + 2\eta^y_\alpha \lambda^z_\alpha 1_\alpha - 2\eta^y_\alpha \delta_\alpha \lambda^z_{\alpha'} \delta_{\alpha'} && (4.60)\\
\partial_\ell \epsilon &= -2\Delta\eta^y + 2\eta^z_\alpha \lambda^x_\alpha 1_\alpha + 2\eta^x_\alpha \lambda^y_\alpha 1_\alpha + 2\eta^e_\alpha \lambda^z_\alpha - 2\eta^y_\alpha \delta_\alpha \lambda^x_{\alpha'} \delta_{\alpha'} && (4.61)\\
\partial_\ell \lambda^e_\alpha &= 2\eta^e_\alpha \omega_\alpha + 2\eta^e_{\alpha,\alpha'} \lambda^e_{\alpha'} - 2(\eta^e_{\alpha,\alpha'} \omega_{\alpha'} + \eta^e_{\alpha',\alpha} \omega_\alpha)\delta_{\alpha'} && (4.62)\\
\partial_\ell \lambda^x_\alpha &= -2\epsilon\eta^y_\alpha + 2\eta^x_\alpha \omega_\alpha - 2\eta^y \lambda^z_\alpha + 2\eta^e_{\alpha,\alpha'} \lambda^x_{\alpha'} + 2(\eta^y_\alpha \lambda^z_{\alpha'} + \eta^y_{\alpha'} \lambda^z_\alpha)\delta_{\alpha'} && (4.63)\\
\partial_\ell \lambda^y_\alpha &= -2\Delta\eta^z_\alpha - 2\epsilon\eta^x_\alpha + 2\eta^y_\alpha \omega_\alpha - 2\eta^e_{\alpha',\alpha} \lambda^y_{\alpha'} - 2(\eta^z_\alpha \lambda^x_{\alpha'} - \eta^x_\alpha \lambda^z_{\alpha'})\delta_{\alpha'} && (4.64)\\
\partial_\ell \lambda^z_\alpha &= -2\Delta\eta^y_\alpha + 2\eta^z_\alpha \omega_\alpha + 2\eta^y \lambda^x_\alpha + 2\eta^e_{\alpha,\alpha'} \lambda^z_{\alpha'} - 2(\eta^y_\alpha \lambda^x_{\alpha'} + \eta^y_{\alpha'} \lambda^x_\alpha)\delta_{\alpha'} && (4.65)\\
\partial_\ell E &= \eta^x_\alpha \lambda^x_\alpha + \eta^y_\alpha \lambda^y_\alpha + \eta^z_\alpha \lambda^z_\alpha - \eta^e_{\alpha,\alpha'} \omega_{\alpha'} \delta_\alpha \delta_{\alpha'} && (4.66)
\end{aligned}
$$

We introduced the displacement of the distinguished position operator $\bar{x}_\alpha = x_\alpha + \delta_\alpha$ with $\delta_\alpha \equiv \langle\sigma_i\rangle \frac{\lambda^i_\alpha}{\omega_\alpha}$ and the factor $1_\alpha \equiv (1 + 2n_\alpha)$ that stems from normal ordering, $n_\alpha \equiv (e^{\beta\omega_\alpha} - 1)^{-1}$ being the Bose factor.

[5] Summation over α of the terms $\eta^j_\alpha \omega_\alpha$ with $j = e, x, y, z$ in Eqs. (4.62) - (4.65) and $\eta^e_{\alpha',\alpha}\omega_\alpha$ in Eq. (4.62) is not implied.

This is the general version of our Flow Equation. We are still free to choose the constants of the generator η. The only requirement we have so far is that the system should be decoupled from the bath for $\ell \to \infty$. We are also free to choose the distinct expectation values of the system variables.

We now want to impose another obvious condition on the choice of the constants of the generator. They shall be chosen in such a way that the error made by neglecting the operators $\mathcal{O}_i$, $i = 1..7$ is small. One way to do so is to also normal order the system operators and choose the parameters $\eta^e_{\alpha,\alpha'}$ such that the normal ordered bosonic bilinears, that only couple to unity of the two-dimensional Hilbert space, vanish. We thus obtain

$$\begin{aligned}\eta^e_{\alpha,\alpha'} = -(\omega_\alpha^2 - \omega_{\alpha'}^2)^{-1}(\omega_\alpha(\langle\sigma_x\rangle(\eta^z_\alpha\lambda^y_{\alpha'} + \eta^z_{\alpha'}\lambda^y_\alpha) - \langle\sigma_z\rangle(\eta^x_\alpha\lambda^y_{\alpha'} + \eta^x_{\alpha'}\lambda^y_\alpha))\\ +\omega_{\alpha'}(\langle\sigma_x\rangle(\eta^y_\alpha\lambda^z_{\alpha'} + \eta^y_{\alpha'}\lambda^z_\alpha) - \langle\sigma_z\rangle(\eta^y_\alpha\lambda^x_{\alpha'} + \eta^y_{\alpha'}\lambda^x_\alpha))) \quad .\end{aligned} \tag{4.67}$$

To determine the other parameters, there are many possibilities as was pointed out in Chapter 3. For example they can be determined according to the canonical generator $\eta = [H_0, H]$ with suitable H_0.

Another approach is to demand the from-invariance of the initial Hamiltonian given in Eq. (4.41), i.e. $\lambda^e_\alpha = \lambda^x_\alpha = \lambda^y_\alpha = 0$ for all ℓ. This leads to further conditions for the parameters of the generator. If no bias ϵ is present the constants are determined up to a function f_α, see last section. This freedom allows for an improvement of the flow of the parameters by making the neglected operators more irrelevant. If a bias ϵ is present the constants of the generator are determined up to a factor which will set the scale of the ℓ-flow.

In the following we want to allow a bias to be present. If one chooses the free factor such that $\eta^y = \epsilon\Delta/2 - \langle\sigma_z\rangle\Delta\widetilde{\Lambda}$ one finds that $\eta^e_\alpha = 2\langle\sigma_x\rangle\langle\sigma_z\rangle\eta^y_\alpha\widetilde{\Lambda}/\omega_\alpha$, $\eta^x_\alpha = 0$, $\eta^y_\alpha = -\Delta\lambda^z_\alpha/2$, $\eta^z_\alpha = -\omega_\alpha\lambda^z_\alpha/2$ and $\eta^e_{\alpha,\alpha'} = \Delta\langle\sigma_x\rangle\lambda^z_\alpha\lambda^z_{\alpha'}\omega_{\alpha'}/(\omega_\alpha^2 - \omega_{\alpha'}^2)$, where we introduced $\widetilde{\Lambda} \equiv \frac{\lambda^z_\alpha\lambda^z_\alpha}{\omega_\alpha}$.

Defining the spectral function

$$J(\omega) = \sum_\alpha \lambda_\alpha^2\delta(\omega - \omega_\alpha) \quad , \tag{4.68}$$

one obtains the following coupled integro-differential equations:

$$\partial_\ell\Delta = -\Delta\int d\omega J(\omega,\ell)(2n(\omega)+1) + \Delta(\epsilon - \langle\sigma_z\rangle\widetilde{\Lambda})^2 \tag{4.69}$$

$$\partial_\ell\epsilon = -\Delta^2\epsilon + 2\langle\sigma_z\rangle\Delta^2\widetilde{\Lambda} - 2\langle\sigma_z\rangle\langle\sigma_x\rangle\Delta\widetilde{\Lambda}^2 \tag{4.70}$$

$$\partial_\ell J(\omega,\ell) = 2J(\omega,\ell)(\Delta^2 - \omega^2) + 4\Delta\langle\sigma_x\rangle J(\omega,\ell)\int d\omega'\frac{J(\omega',\ell)\omega'}{\omega^2 - \omega'^2} \tag{4.71}$$

These are the same Flow Equations as given in Appendix D where they are set up for a Hamiltonian exhibiting no explicit reflection symmetry. This indicates that this approach is invariant of the representation of the initial Hamiltonian.

The Flow Equations still depend on the expectation values of the system variables. The most straightforward way is to evaluate them with respect to the effective one-particle Hamiltonian as was done in Section 3 and in Appendix D.

Another possibility is to solve the set of self-consistent equations given in Eq. (4.48). In case of the form-invariant Hamiltonian ($\lambda_\alpha^e = \lambda_\alpha^x = \lambda_\alpha^y = 0$), the set reduces to one self-consistent equation:

$$\langle \sigma_z \rangle = -\frac{\epsilon - \langle \sigma_z \rangle \widetilde{\Lambda}}{\sqrt{\Delta^2 + (\epsilon - \langle \sigma_z \rangle \widetilde{\Lambda})^2}} \tag{4.72}$$

This leads us to the problem of finding the roots of the polynomial $P(z) = (z - \epsilon/\widetilde{\Lambda})^2(z+1)(z-1) + (\Delta/\widetilde{\Lambda})^2 z^2$.

If no bias ϵ is applied in the initial Hamiltonian the self-consistent equation can be readily solved. We always obtain the double root $\langle \sigma_z \rangle = 0$ and thus $\langle \sigma_x \rangle = 1$. But if $\widetilde{\Lambda} > \Delta$ we also get $\langle \sigma_z \rangle = \pm\sqrt{\widetilde{\Lambda}^2 - \Delta^2}/\widetilde{\Lambda}$ and thus $\langle \sigma_x \rangle = \Delta/\widetilde{\Lambda}$. We want to point out that any solution implies that there is no flow of the bias ϵ, i.e. $\epsilon = 0$ for all ℓ.

Let us analyze the Flow Equations for small, but finite bias. Expanding $\langle \sigma_z \rangle$ and $\langle \sigma_x \rangle$ around the two different solutions of the self-consistent equation obtained for $\epsilon = 0$, we find that for $\langle \sigma_z \rangle \approx 0$ the line $\epsilon = 0$ is unstable at $\ell = 0$ since $\partial_\ell \epsilon \to 2\widetilde{\Lambda}^2 \epsilon$, see also Appendix D. But for $\langle \sigma_z \rangle \approx \pm\sqrt{\widetilde{\Lambda}^2 - \Delta^2}/\widetilde{\Lambda}$ the line $\epsilon = 0$ becomes stable at $\ell = 0$ since $\partial_\ell \epsilon \to -3\Delta^2 \epsilon$. This shows that the one-particle expectation values can significantly alter the behaviour of the Flow Equations.

4.3.2. Flow Equations for Observables

We will now investigate the flow of the observables. The z-component of the Pauli spin matrices as a function of the flow parameter ℓ shall be given by[6]

$$\begin{aligned} \sigma_z(\ell) &= g(\ell)\sigma_x + h(\ell)\sigma_z + f(\ell) + \sigma_i \chi_\alpha^i \bar{x}_\alpha + i\sigma_y \chi_\alpha^y \bar{p}_\alpha \\ &+ \psi_{\alpha,\alpha'}^+ : \bar{x}_\alpha \bar{x}_{\alpha'} : + \psi_{\alpha,\alpha'}^- : \bar{p}_\alpha \bar{p}_{\alpha'} : \quad . \end{aligned} \tag{4.73}$$

We have to transform the observables by the same sequence of infinitesimal transformations by which we have transformed the Hamiltonian, i.e. $\partial_\ell \sigma_z = [\eta, \sigma_z]$. Then we can take advantage of the simple structure of $H(\ell = \infty)$. Notice that there is also a ℓ-dependence of $\bar{x}_\alpha$ since the operator contains the ℓ-dependent shift δ_α. The transformation of the observable can therefore be considered active *and* passive.

[6] The flow of σ_x only differs from the initial condition.

The commutator $[\eta, \sigma_z]$ yields the following contributions:

$$
\begin{aligned}
[\eta^{y,0}, \sigma_z(\ell)] &= 2g\eta^y\sigma_z - 2h\eta^y\sigma_x + 2\sigma_z\eta^y\chi^x_\alpha\bar{x}_\alpha - 2\eta^y\sigma_x\chi^z_\alpha\bar{x}_\alpha & (4.74)\\
[\eta^{e,1}, \sigma_z(\ell)] &= 2\eta^e_\alpha\chi^e_\alpha + 2\sigma_x\eta^e_\alpha\chi^x_\alpha + 2\sigma_z\eta^e_\alpha\chi^z_\alpha + 2\eta^e_{\alpha'}(\psi^+_{\alpha,\alpha'} + \psi^+_{\alpha,\alpha'})\bar{x}_\alpha & (4.75)\\
[\eta^{x,1}, \sigma_z(\ell)] &= -2i\sigma_y h\eta^x_\alpha p_\alpha + 2\sigma_x\eta^x_\alpha\chi^e_\alpha + 2\eta^x_\alpha\chi^x_\alpha - 2\sigma_z\eta^x_\alpha\chi^y_{\alpha'}p_\alpha\bar{p}_{\alpha'}\\
&\quad - i\sigma_y\eta^x_\alpha\chi^z_{\alpha'}\{p_\alpha, \bar{x}_{\alpha'}\} + 2\sigma_x\eta^x_{\alpha'}(\psi^+_{\alpha,\alpha'} + \psi^+_{\alpha',\alpha})\bar{x}_\alpha & (4.76)\\
[\eta^{y,1}, \sigma_z(\ell)] &= 2g\sigma_z\eta^y_\alpha x_\alpha - 2h\sigma_x\eta^y_\alpha x_\alpha + 2\sigma_z\eta^y_\alpha\chi^x_{\alpha'}x_\alpha\bar{x}_{\alpha'}\\
&\quad + 2\eta^y_\alpha\chi^y_\alpha - 2\sigma_x\eta^y_\alpha\chi^z_{\alpha'}x_\alpha\bar{x}_{\alpha'} + 2 - 2i\sigma_y\eta^y_{\alpha'}(\psi^-_{\alpha,\alpha'} + \psi^-_{\alpha',\alpha})\bar{p}_\alpha & (4.77)\\
[\eta^{z,1}, \sigma_z(\ell)] &= 2gi\sigma_y\eta^z_\alpha p_\alpha + 2\sigma_z\eta^z_\alpha\chi^e_\alpha + i\sigma_y\eta^z_\alpha\chi^x_{\alpha'}\{p_\alpha, \bar{x}_{\alpha'}\}\\
&\quad + 2\sigma_x\eta^z_\alpha\chi^y_{\alpha'}p_\alpha\bar{p}_{\alpha'} + 2\eta^z_\alpha\chi^z_\alpha + 2\sigma_z\eta^z_{\alpha'}(\psi^+_{\alpha,\alpha'} + \psi^+_{\alpha',\alpha})\bar{x}_\alpha & (4.78)\\
[\eta^{e,2}, \sigma_z(\ell)] &= 2\eta^e_{\alpha,\alpha'}\chi^e_{\alpha'}x_\alpha + 2\sigma_x\eta^e_{\alpha,\alpha'}\chi^x_{\alpha'}x_\alpha - 2i\sigma_y\eta^e_{\alpha,\alpha'}\chi^y_\alpha p_{\alpha'}\\
&\quad + 2\sigma_z\eta^e_{\alpha,\alpha'}\chi^z_{\alpha'}x_\alpha + 2\eta^e_{\alpha,\alpha''}(\psi^+_{\alpha',\alpha''} + \psi^+_{\alpha'',\alpha'})x_\alpha\bar{x}_{\alpha'} & (4.79)\\
&\quad + 2\eta^e_{\alpha'',\alpha}(\psi^-_{\alpha',\alpha''} + \psi^-_{\alpha'',\alpha'})p_\alpha\bar{p}_{\alpha'} \quad .
\end{aligned}
$$

Again the Flow Equations do not close and we will have to neglect normal ordered bosonic bilinears:

$$
\begin{aligned}
\mathcal{O}_1 &= - :\sigma_x:\eta^y_\alpha\chi^z_{\alpha'}:\bar{x}_\alpha\bar{x}_{\alpha'}: \quad , \quad \mathcal{O}_2 =:\sigma_z:\eta^y_\alpha\chi^x_{\alpha'}:\bar{x}_\alpha\bar{x}_{\alpha'}: \quad , & (4.80)\\
\mathcal{O}_3 &=:\sigma_x:\eta^z_\alpha\chi^y_{\alpha'}:\bar{p}_\alpha\bar{p}_{\alpha'}: \quad , \quad \mathcal{O}_4 = - :\sigma_z:\eta^x_\alpha\chi^y_{\alpha'}:\bar{p}_\alpha\bar{p}_{\alpha'}: \quad , & (4.81)\\
\mathcal{O}_5 &= i\sigma_y(\eta^z_\alpha\frac{\chi^x_{\alpha'}}{2} - \eta^x_\alpha\frac{\lambda^z_{\alpha'}}{2}) : \{\bar{p}_\alpha, \bar{x}_{\alpha'}\} : \quad . & (4.82)
\end{aligned}
$$

With $\delta_\alpha = \langle\sigma_i\rangle\lambda^i_\alpha/\omega_\alpha$ and $\tilde{\psi}^\pm_{\alpha,\alpha'} \equiv (\psi^\pm_{\alpha,\alpha'} + \psi^\pm_{\alpha',\alpha})/2$ this yields the following Flow

Equations:

$$\begin{aligned}
\partial_\ell g &= -2h\eta^y + 2\eta^x_\alpha\chi^e_\alpha + 2\eta^e_\alpha\chi^x_\alpha - 2\eta^z_\alpha\chi^y_\alpha 1_\alpha - 2\eta^y_\alpha\chi^z_\alpha 1_\alpha \\
&\quad + 2h\eta^y_\alpha\delta_\alpha - 2\eta^e_{\alpha,\alpha'}\chi^x_{\alpha'}\delta_\alpha - \chi^x_\alpha\partial_\ell\delta_\alpha && (4.83)\\
\partial_\ell h &= 2g\eta^y + 2\eta^z_\alpha\chi^e_\alpha + 2\eta^y_\alpha\chi^x_\alpha 1_\alpha + 2\eta^x_\alpha\chi^y_\alpha 1_\alpha + 2\eta^e_\alpha\chi^z_\alpha \\
&\quad - 2g\eta^y_\alpha\delta_\alpha - 2\eta^e_{\alpha,\alpha'}\chi^z_{\alpha'}\delta_\alpha - \chi^z_\alpha\partial_\ell\delta_\alpha && (4.84)\\
\partial_\ell f &= 2(\eta^e_\alpha\chi^e_\alpha + \eta^x_\alpha\chi^x_\alpha + \eta^y_\alpha\chi^y_\alpha + \eta^z_\alpha\chi^z_\alpha) - 2\eta^e_{\alpha,\alpha'}\chi^e_{\alpha'}\delta_\alpha + 4\eta^e_{\alpha,\alpha'}\tilde{\psi}^+_{\alpha',\alpha}1_\alpha && (4.85)\\
&\quad - 4\eta^e_{\alpha,\alpha'}\tilde{\psi}^-_{\alpha',\alpha}1_\alpha - \chi^e_\alpha\partial_\ell\delta_\alpha \\
\partial_\ell\chi^e_\alpha &= 4\eta^e_{\alpha'}\tilde{\psi}^+_{\alpha',\alpha} + 2\eta^e_{\alpha,\alpha'}\chi^e_{\alpha'} - 4\eta^e_{\alpha',\alpha''}\tilde{\psi}^+_{\alpha'',\alpha}\delta_{\alpha'} - 2\tilde{\psi}^+_{\alpha,\alpha'}\partial_\ell\delta_{\alpha'} && (4.86)\\
\partial_\ell\chi^x_\alpha &= -2h\eta^y_\alpha - 2\eta^y\chi^z_\alpha + 2\eta^e_{\alpha,\alpha'}\chi^x_{\alpha'} + 2\eta^x_{\alpha'}\tilde{\psi}^+_{\alpha',\alpha} + 2\eta^y_{\alpha'}\chi^z_\alpha\delta_{\alpha'} && (4.87)\\
\partial_\ell\chi^y_\alpha &= 2g\eta^z_\alpha - 2h\eta^x_\alpha - 2\eta^e_{\alpha',\alpha}\chi^y_{\alpha'} - 2\eta^y_{\alpha'}\tilde{\psi}^-_{\alpha',\alpha} && (4.88)\\
\partial_\ell\chi^z_\alpha &= 2g\eta^y_\alpha + 2\eta^y\chi^x_\alpha + 2\eta^e_{\alpha,\alpha'}\chi^z_{\alpha'} + 2\eta^z_{\alpha'}\tilde{\psi}^+_{\alpha',\alpha} - 2\eta^y_{\alpha'}\chi^x_\alpha\delta_{\alpha'} && (4.89)\\
\partial_\ell\tilde{\psi}^+_{\alpha,\alpha'} &= \langle\sigma_z\rangle(\eta^y_\alpha\chi^x_{\alpha'} + \eta^y_{\alpha'}\chi^x_\alpha) - \langle\sigma_x\rangle(\eta^y_\alpha\chi^z_{\alpha'} + \eta^y_{\alpha'}\chi^z_\alpha) \\
&\quad - 2(\eta^e_{\alpha'',\alpha}\tilde{\psi}^+_{\alpha'',\alpha'} + \eta^e_{\alpha'',\alpha'}\tilde{\psi}^+_{\alpha'',\alpha}) && (4.90)\\
\partial_\ell\tilde{\psi}^-_{\alpha,\alpha'} &= \langle\sigma_x\rangle(\eta^z_\alpha\chi^y_{\alpha'} + \eta^z_{\alpha'}\chi^y_\alpha) - \langle\sigma_z\rangle(\eta^x_\alpha\chi^y_{\alpha'} + \eta^x_{\alpha'}\chi^y_\alpha) \\
&\quad - 2(\eta^e_{\alpha'',\alpha}\tilde{\psi}^-_{\alpha'',\alpha'} + \eta^e_{\alpha'',\alpha'}\tilde{\psi}^-_{\alpha'',\alpha}) && (4.91)
\end{aligned}$$

In the first four equations of the above set contributions of the form $\chi^i_\alpha\partial_\ell\delta_\alpha$ appear that stem form the ℓ-dependence of $\bar{x}_\alpha$. The differential equation for $\delta_\alpha = \langle\sigma_i\rangle\lambda^i_\alpha/\omega$ is obtained from the Flow Equations (4.60) - (4.66) and from the explicit realization of the one-particle expectation values.

Choosing the constants of the generator such that the Hamiltonian remains form-invariant and setting $\epsilon = 0$ and $\langle\sigma_z\rangle = 0$, the above Flow Equations simplify considerably:

$$\begin{aligned}
\partial_\ell h &= -\Delta\lambda^z_\alpha\chi^x_\alpha 1_\alpha \\
\partial_\ell\chi^x_\alpha &= \Delta\lambda^z_\alpha h + 2\Delta\langle\sigma_x\rangle\lambda^z_\alpha\frac{\lambda^z_{\alpha'}\chi^x_{\alpha'}\omega_{\alpha'}}{\omega^2_\alpha - \omega^2_{\alpha'}}
\end{aligned} \tag{4.92}$$

We will study these Flow Equations in order to demonstrate their universal asymptotic behaviour. But the sum rule $\sigma_z^2 = 1$ is not fulfilled since the above equations yield for $T = 0$

$$\partial_\ell\langle\sigma_z^2\rangle = \partial_\ell(h^2 + (\chi^x_\alpha)^2) = -2\Delta\langle\sigma_x\rangle\frac{\lambda^z_\alpha\chi^x_\alpha\lambda^z_{\alpha'}\chi^x_{\alpha'}}{\omega_\alpha + \omega_{\alpha'}} \quad . \tag{4.93}$$

This means that the spectral function $C(\omega) \equiv (\chi^x_\alpha)^2\delta(\omega - \omega_\alpha)$ does not fulfill the spectral sum rule $\int d\omega C(\omega) = 1$ either.[7]

[7] Remember that $h \to 0$ for $\ell \to \infty$.

If the reflection symmetry is broken the flow of σ_z is not restricted to this subspace anymore that only involves the parameters h and χ^x_α. The sum rule $\sigma_z^2 = 1$ then reads

$$\begin{aligned}\langle\sigma_z^2(\ell)\rangle &= g^2 + h^2 + f^2 + (\chi^x_\alpha\chi^x_\alpha + \chi^y_\alpha\chi^y_\alpha + \chi^z_\alpha\chi^z_\alpha)1_\alpha \\ &+ 2(\langle\sigma_x\rangle g + \langle\sigma_z\rangle h)f + 2(\langle\sigma_z\rangle\chi^x_\alpha\chi^y_\alpha - \langle\sigma_x\rangle\chi^y_\alpha\chi^z_\alpha) \approx 1 \quad .\end{aligned} \tag{4.94}$$

Under the premise $g(\ell = \infty) = 0$ and $h(\ell = \infty) = 0$ the symmetrized equilibrium correlation function reads

$$\begin{aligned}C(\omega) &= f^2\delta(\omega) + (\chi^x_\alpha\chi^x_\alpha + \chi^y_\alpha\chi^y_\alpha + \chi^z_\alpha\chi^z_\alpha)1_\alpha\delta(\omega - \omega_\alpha) \\ &+ 2(\langle\sigma_z\rangle\chi^x_\alpha\chi^y_\alpha - \langle\sigma_x\rangle\chi^z_\alpha\chi^y_\alpha)\delta(\omega - \omega_\alpha) \quad .\end{aligned} \tag{4.95}$$

The expectation value of σ_z with respect to the entire Hamiltonian is given by $\langle\sigma_z\rangle = f^*$ with $f^* \equiv f(\ell = \infty)$. In order to describe the phase transition one thus has to employ the extended truncation scheme to allow for a finite expectation value $\langle\sigma_z\rangle \neq 0$.

We want to note that one can determine the expectation values such that the flow of the Hamiltonian is coupled to the flow of the observables. The expectation value $\langle\sigma_z\rangle$ is then determined by the differential equation stemming from the condition $\partial_\ell\langle\sigma_z^2\rangle = 0$ and setting $\langle\sigma_x\rangle = \sqrt{1 - \langle\sigma_z\rangle^2}$. Defining $\partial_\ell\tilde{g} \equiv \partial_\ell g + (\partial_\ell\langle\sigma_i\rangle)\lambda^i_\alpha\chi^x_\alpha/\omega_\alpha$ and $\partial_\ell\tilde{h} \equiv \partial_\ell h + (\partial_\ell\langle\sigma_i\rangle)\lambda^i_\alpha\chi^z_\alpha/\omega_\alpha$, we thus obtain $\partial_\ell\langle\sigma_z\rangle = A/B$ with:

$$\begin{aligned}A &\equiv g\partial_\ell\tilde{g} + h\partial_\ell\tilde{h} + f\partial_\ell f + \chi^x_\alpha\partial_\ell\chi^x_\alpha + \chi^y_\alpha\partial_\ell\chi^y_\alpha + \chi^z_\alpha\partial_\ell\chi^z_\alpha \\ &+ \langle\sigma_x\rangle f\partial_\ell\tilde{g} + \langle\sigma_z\rangle f\partial_\ell\tilde{h} + \langle\sigma_x\rangle g\partial_\ell f + \langle\sigma_z\rangle h\partial_\ell f + \langle\sigma_z\rangle\partial_\ell(\chi^x_\alpha\chi^y_\alpha) - \langle\sigma_x\rangle\partial_\ell(\chi^y_\alpha\chi^z_\alpha)\end{aligned} \tag{4.96}$$

$$\begin{aligned}B &\equiv (g + \langle\sigma_x\rangle f)\frac{\lambda^z_\alpha\chi^x_\alpha}{\omega_\alpha} + (h + \langle\sigma_z\rangle f)\frac{\lambda^z_\alpha\chi^z_\alpha}{\omega_\alpha} - hf - \chi^x_\alpha\chi^y_\alpha \\ &- \langle\sigma_z\rangle/\langle\sigma_x\rangle((g + \langle\sigma_x\rangle f)\frac{\lambda^x_\alpha\chi^x_\alpha}{\omega_\alpha} + (h + \langle\sigma_z\rangle f)\frac{\lambda^x_\alpha\chi^z_\alpha}{\omega_\alpha} - gf + \chi^y_\alpha\chi^z_\alpha)\end{aligned} \tag{4.97}$$

Since $B(\ell = 0) = 0$ the differential equation only holds for $\ell > 0$. Another possibility to couple the flow of the Hamiltonian and the flow of the observables is to also include the flow of σ_x and determine the expectation value $\langle\sigma_x\rangle$ through the condition $\partial_\ell\langle\sigma_x^2\rangle = 0$.

We close this section with the explicit differential equations of the observable flow choosing the parameters of the generator that induce the form-invariant flow of the Hamiltonian. For the parameters of the operators acting on the two-dimensional

Hilbert space we obtain:

$$\partial_\ell g = -\epsilon\Delta h + \omega_\alpha\lambda^z_\alpha\chi^y_\alpha 1_\alpha + \Delta\lambda^z_\alpha\chi^z_\alpha 1_\alpha - h\Delta\langle\sigma_z\rangle\frac{\lambda^z_\alpha\lambda^z_\alpha}{\omega_\alpha}$$
$$+\,\epsilon\Delta\langle\sigma_z\rangle\frac{\lambda^z_\alpha\chi^z_\alpha}{\omega_\alpha} + \langle\sigma_z\rangle\Delta^2\frac{\lambda^z_\alpha\chi^x_\alpha}{\omega_\alpha} - \langle\sigma_z\rangle\omega_\alpha\lambda_\alpha\chi^x_\alpha - (\partial_\ell\langle\sigma_z\rangle)\frac{\lambda^z_\alpha\chi^x_\alpha}{\omega_\alpha} \tag{4.98}$$

$$\partial_\ell h = \epsilon\Delta g - \omega_\alpha\lambda^z_\alpha\chi^e_\alpha 1_\alpha - \Delta\lambda^z_\alpha\chi^x_\alpha 1_\alpha - g\Delta\langle\sigma_z\rangle\frac{\lambda^z_\alpha\lambda^z_\alpha}{\omega_\alpha}$$
$$-\,\epsilon\Delta\langle\sigma_z\rangle\frac{\lambda^z_\alpha\chi^x_\alpha}{\omega_\alpha} + \langle\sigma_z\rangle\Delta^2\frac{\lambda^z_\alpha\chi^z_\alpha}{\omega_\alpha} - \langle\sigma_z\rangle\omega_\alpha\lambda_\alpha\chi^z_\alpha - (\partial_\ell\langle\sigma_z\rangle)\frac{\lambda^z_\alpha\chi^z_\alpha}{\omega_\alpha} \tag{4.99}$$

$$\partial_\ell f = -\Delta\lambda^z_\alpha\chi^y_\alpha - \omega_\alpha\lambda^z_\alpha\chi^z_\alpha + \langle\sigma_z\rangle\Delta^2\frac{\lambda^z_\alpha\chi^e_\alpha}{\omega_\alpha} - \langle\sigma_z\rangle\omega_\alpha\lambda_\alpha\chi^e_\alpha - (\partial_\ell\langle\sigma_z\rangle)\frac{\lambda^z_\alpha\chi^e_\alpha}{\omega_\alpha}$$
$$+\,4\Delta\langle\sigma_x\rangle\frac{\lambda^z_\alpha\lambda^z_{\alpha'}\omega_{\alpha'}\tilde{\psi}^+_{\alpha',\alpha}}{\omega^2_\alpha-\omega^2_{\alpha'}} - 4\Delta\langle\sigma_x\rangle\frac{\lambda^z_\alpha\lambda^z_{\alpha'}\omega_{\alpha'}\tilde{\psi}^-_{\alpha',\alpha}}{\omega^2_\alpha-\omega^2_{\alpha'}} \tag{4.100}$$

The Flow Equations for the bath operators read:

$$\partial_\ell\chi^e_\alpha = -4\langle\sigma_x\rangle\langle\sigma_z\rangle\Delta\widetilde{\Lambda}\frac{\lambda^z_{\alpha'}\tilde{\psi}^+_{\alpha',\alpha}}{\omega_{\alpha'}} + 2\Delta\langle\sigma_x\rangle\lambda^z_\alpha\frac{\lambda^z_{\alpha'}\chi^e_{\alpha'}\omega_{\alpha'}}{\omega^2_\alpha-\omega^2_{\alpha'}}$$
$$-\,4\Delta\langle\sigma_x\rangle\langle\sigma_z\rangle\frac{\lambda^z_{\alpha'}\lambda^z_{\alpha'}}{\omega_{\alpha'}}\frac{\lambda^z_{\alpha''}\tilde{\psi}^+_{\alpha'',\alpha}}{\omega^2_{\alpha'}-\omega^2_{\alpha''}} - 2\tilde{\psi}^+_{\alpha,\alpha'}\partial_\ell\delta_{\alpha'} \tag{4.101}$$

$$\partial_\ell\chi^x_\alpha = \Delta\lambda^z_\alpha h - \epsilon\Delta\chi^z_\alpha + 2\Delta\langle\sigma_x\rangle\lambda^z_\alpha\frac{\lambda^z_{\alpha'}\chi^x_{\alpha'}\omega_{\alpha'}}{\omega^2_\alpha-\omega^2_{\alpha'}} - \Delta\chi^z_\alpha\langle\sigma_z\rangle\frac{\lambda^z_{\alpha'}\lambda^z_{\alpha'}}{\omega_{\alpha'}} \tag{4.102}$$

$$\partial_\ell\chi^y_\alpha = -\omega_\alpha\lambda^z_\alpha g - 2\Delta\langle\sigma_x\rangle\lambda^z_\alpha\frac{\lambda^z_{\alpha'}\chi^y_{\alpha'}\omega_{\alpha'}}{\omega^2_\alpha-\omega^2_{\alpha'}} + \Delta\lambda^z_{\alpha'}\tilde{\psi}^-_{\alpha',\alpha} \tag{4.103}$$

$$\partial_\ell\chi^z_\alpha = -\Delta\lambda^z_\alpha g + \epsilon\Delta\chi^x_\alpha + 2\Delta\langle\sigma_x\rangle\lambda^z_\alpha\frac{\lambda^z_{\alpha'}\chi^z_{\alpha'}\omega_{\alpha'}}{\omega^2_\alpha-\omega^2_{\alpha'}} - \Delta\chi^x_\alpha\langle\sigma_z\rangle\frac{\lambda^z_{\alpha'}\lambda^z_{\alpha'}}{\omega_{\alpha'}} \tag{4.104}$$

$$\partial_\ell\tilde{\psi}^+_{\alpha,\alpha'} = -\langle\sigma_z\rangle\frac{\Delta}{2}(\lambda^z_\alpha\chi^x_{\alpha'} + \lambda^z_{\alpha'}\chi^x_\alpha) + +\langle\sigma_x\rangle\frac{\Delta}{2}(\lambda^z_\alpha\chi^z_{\alpha'} + \lambda^z_{\alpha'}\chi^z_\alpha)$$
$$-\,2\Delta\langle\sigma_x\rangle\left(\frac{\lambda^z_\alpha\lambda^z_{\alpha''}\tilde{\psi}^+_{\alpha'',\alpha'}\omega_\alpha}{\omega^2_{\alpha''}-\omega^2_\alpha} + \frac{\lambda^z_{\alpha'}\lambda^z_{\alpha''}\tilde{\psi}^+_{\alpha'',\alpha}\omega_{\alpha'}}{\omega^2_{\alpha''}-\omega^2_{\alpha'}}\right) \tag{4.105}$$

$$\partial_\ell\tilde{\psi}^-_{\alpha,\alpha'} = -\langle\sigma_z\rangle\frac{\Delta}{2}(\lambda^y_\alpha\chi^x_{\alpha'} + \lambda^y_{\alpha'}\chi^x_\alpha)$$
$$-\,2\Delta\langle\sigma_x\rangle\left(\frac{\lambda^z_\alpha\lambda^z_{\alpha''}\tilde{\psi}^-_{\alpha'',\alpha'}\omega_\alpha}{\omega^2_{\alpha''}-\omega^2_\alpha} + \frac{\lambda^z_{\alpha'}\lambda^z_{\alpha''}\tilde{\psi}^-_{\alpha'',\alpha}\omega_{\alpha'}}{\omega^2_{\alpha''}-\omega^2_{\alpha'}}\right) \tag{4.106}$$

4.3.3. Universal Asymptotic Behaviour

In this subsection we will derive differential equations which govern the asymptotic spectral functions and the asymptotic flow of the observable. The procedure outlined here is closely related to the one discussed in subsection 2.3.2.

The asymptotic Flow Equations for the Spin-Boson Model shall reduce to

$$\partial_\ell \Delta = -\Delta \int d\omega J(\omega,\ell) \tag{4.107}$$

$$\partial_\ell J(\omega,\ell) = 2J(\omega,\ell)(\Delta^2-\omega^2) + 4\Delta J(\omega,\ell)\int d\omega' \frac{J(\omega',\ell)\omega'}{\omega^2-\omega'^2} \quad . \tag{4.108}$$

We now make the ansatz $\Delta \to a\ell^{-1/2}$ and $\widetilde{\Lambda}(\ell) \to b\ell^{-1/2}$ with $\widetilde{\Lambda}(\ell) \equiv \int d\omega J(\omega,\ell)/\omega$ as $\ell \to \infty$. We further parameterize the asymptotic spectral function by one parameter s, i.e. we assume that $J(\omega,\ell) \to \omega^s \hat{J}(\ell)\bar{J}(y)$, where $y \equiv \omega\sqrt{\ell}$ and $\bar{J}(y) \to J_0$ for $y \to 0$. Notice that we dropped the index s on the functions $J(\omega,\ell)$, $\hat{J}(\ell)$ and $\bar{J}(y)$.

The differential equation for $\widetilde{\Lambda}$ is given by

$$\partial_\ell \widetilde{\Lambda} = 2\widetilde{\Lambda}\Delta^2 - 2\int d\omega J(\omega,\ell)\omega - 2\Delta\widetilde{\Lambda}^2 \quad . \tag{4.109}$$

The differential equation for $\hat{J}(\ell)$ is obtained from Eq. (4.108) by setting $\omega = 0$ and yields

$$\partial_\ell \hat{J}(\ell) = \hat{J}(\ell)(2\Delta^2 - 4\Delta\widetilde{\Lambda}) \quad . \tag{4.110}$$

Comparing the asymptotic behaviour that follows from the differential equations of $\widetilde{\Lambda}$ and Δ with the above ansatz, one obtains self-consistency if $\hat{J}(\ell) \to \ell^{(s-1)/2}$. From Eq. (4.110) it then follows that $2a^2 - 4ab = (s-1)/2$. We thus obtain $a = b + \sqrt{b^2 + (s-1)/4}$.[8]

With the relation for the constants a and b, we obtain the following non-local differential equation for $J(y) \equiv y^{s-1}\bar{J}(y)$:

$$\partial_y J(y) = -4yJ(y)(1 - 2a\int_0^\infty dy' \frac{J(y')}{y^2 - y'^2}) + (s-1)\frac{J(y)}{y} \tag{4.111}$$

With the above ansatz for the asymptotic behaviour the system will be thus decoupled from the bath since the support of the spectral function vanishes as $\ell^{-1/2}$ and $J(y) \to y^{4a^2}e^{-2y^2}$ for $y \to \infty$. There is thus a *universal* fixed point for all initial tunnel-matrix elements Δ. They are all mapped onto the free bath. For $y \to 0$, Eq. (4.111) yields $J(y) \to J_0 y^{s-1}$.

[8] The minus-sign in the solution of the quadratic equation would yield $a = 0$ in the case of $s = 1$. Therefore, we choose the plus-sign.

Let us briefly discuss this differential equation for the special case $s = 1$. We first neglect the linear term in Eq. (4.111). A solution is then given by $J(y) = \text{const.}$ Further understanding can be obtained by the following (non-systematic) perturbative approach: We first assume that $J(\omega, \ell)$ is analytic in ℓ so that $J(y)$ is an even function. We then have

$$\int_0^\infty dy' \frac{J(y')}{y^2 - y'^2} = \frac{1}{2y} \int_{-\infty}^\infty dy' \frac{J(y')}{y - y'} = -\frac{1}{2} \int_{-\infty}^\infty dy' \frac{J^{(1)}(y')}{y'} + O(y^3) \quad , \tag{4.112}$$

with $J^{(1)}(y) \equiv \partial_y J(y)$. Inserting this expansion into Eq. (4.111) we obtain $J(y) = J_0 \exp(-2y^2/(1+4a^2))$. The two constants J_0 and a are given by the two equations $2\int_0^\infty dy J(y) = a$ and $2\int_0^\infty dy y J(y) = 1$, the first resulting from $a = 2b$ and the latter coming from Eq. (4.107). The non-local term in Eq. (4.111) thus damps the decay of $J(y)$.

To treat Eq. (4.111) exactly one can make the following expansion for $J(y)$:

$$J(y) = \sum_n f_n L_n^{-1/2}(y^2) e^{-y^2} \quad , \tag{4.113}$$

where $L_n^{-1/2}$ denote the associated Laguerre polynomials. Generally they obey the following orthonormal relation:

$$\int_0^\infty dx L_n^\alpha(x) L_m^\alpha(x) x^\alpha e^{-x} = \delta_{n,m} \tag{4.114}$$

First we see that $f_0 = a$ which follows from the relations for a and b. By repeated use of ortho-normality and functional relations of the Laguerre polynomials one can evaluate the y-dependent integral and thus ends up with a non-linear algebraic equation for the coefficients f_n. We did not pursue this further but limited ourself to the numerically self-consistent solution of Eq. (4.111).

Finally we want to mention that the only difference between the asymptotic behaviour of the Dissipative Harmonic Oscillator and the Spin-Boson Model is manifested in the constant a. But in contrary to the exactly solvable Dissipative Harmonic Oscillator this time we cannot determine the value of a since Eq. (4.109) cannot be written as an algebraic equation involving only the constants a and b as it was the case in subsection 2.3.2.

The asymptotic Flow Equations for the observable σ_z shall reduce to

$$\partial_\ell h = -\Delta \int d\omega S(\omega, \ell) \tag{4.115}$$

$$\begin{aligned} \partial_\ell S(\omega, \ell) &= \Delta h J(\omega, \ell) + 2\Delta J(\omega, \ell) \int d\omega' \frac{S(\omega', \ell)\omega'}{\omega^2 - \omega'^2} \\ &+ (\Delta^2 - \omega^2) S(\omega, \ell) + 2\Delta S(\omega, \ell) \int d\omega' \frac{J(\omega', \ell)\omega'}{\omega^2 - \omega'^2} \quad . \end{aligned} \tag{4.116}$$

The above set of equations is obtained from Eqs. (4.92) for $T=0$ by setting $\langle\sigma_x\rangle = 1$ and defining $S(\omega,\ell) \equiv \sum_\alpha \lambda_\alpha \chi_\alpha \delta(\omega - \omega/al)$.

To determine the asymptotic behaviour of $S(\omega,\ell)$ we make a similar ansatz as in the case of the spectral function $J(\omega,\ell)$, namely $h(\ell) \to c\ell^{-s/2}\hat{S}(\ell)$ and $\Sigma(\ell) \to d\ell^{-s/2}\hat{S}(\ell)$ with $\Sigma(\ell) \equiv \int d\omega S(\omega,\ell)/\omega$ as $\ell \to \infty$. Further we assume that $S(\omega,\ell) \to \omega^s \hat{S}(\ell)\bar{S}(y)$, where $y \equiv \omega\sqrt{\ell}$ and $\bar{S}(y) \to S_0$ for $y \to 0$.

The differential equation for Σ is given by

$$\partial_\ell \Sigma = \Delta h \widetilde{\Lambda} + \Delta^2 \Sigma - \int d\omega S(\omega,\ell)\omega - 2\Delta\widetilde{\Lambda}\Sigma \quad . \tag{4.117}$$

The differential equation for $\hat{S}(\ell)$ is obtained from Eq. (4.116) by setting $\omega = 0$. This yields

$$\partial_\ell \hat{S}(\ell) = -\xi \ell^{-(1+s)/2}\hat{S}(\ell) + \frac{s-1}{4}\ell^{-1}\hat{S}(\ell) \quad , \tag{4.118}$$

where we defined $\xi \equiv -(ac - 2ad)J_0/S_0$. For $\ell \to \infty$ we thus obtain $\hat{S}(\ell) \to \ell^{(s-1)/4}$ for $s > 1$, $\hat{S}(\ell) \to \ell^{-\xi}$ for $s = 1$ and $\hat{S}(\ell) \to \exp(-2\xi\ell^{(1-s)/2}/(1-s))$ for $s < 1$. For $s = 1$ we obtain the following non-local differential equation for $S(y) \equiv \bar{S}(y)$:

$$\begin{aligned} \partial_y S(y) = {} & -2yS(y)(1 - 2a\int_0^\infty dy' \frac{J(y')}{y^2 - y'^2}) + 4ayJ(y)\int_0^\infty dy' \frac{S(y')}{y^2 - y'^2} \\ & + 2\xi \frac{S(y) - J(y)S_0/J_0}{y} \end{aligned} \tag{4.119}$$

Eq. (4.119) is linear in $S(y)$. We can therefore not determine the constant S_0 from the asymptotic behaviour. The asymptotic solution of Eq. (2.107) yields $S(y) \to S_0$ for $y \to 0$ and $S(y) \to y^{2a^2}e^{-y^2}$ for $y \to \infty$.

There is one difference to the corresponding differential equation of the Dissipative Harmonic Oscillator given in Eq. (2.107) since the last term is not present in the latter. But since $(S(y) - J(y)S_0/J_0)/y \to 0$ for $y \to 0$, Eq. (4.119) still guarantees that $S(y) \to S_0$ for $y \to 0$.

We want to close this subsection with a remark. Also for Flow Equations with non-universal asymptotic behaviour the asymptotic behaviour can be determined. For Ohmic coupling it yields $\Delta \to \Delta_\infty + \ell^{-1/2}/2$ for coupling constants $\alpha < 1$, with Δ_∞ denoting the renormalized tunnel-matrix element $\Delta_\infty \propto \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$, see Ref. [Keh96b]. For $\alpha > 1$ the asymptotic behaviour is governed by $\Delta \to \ell^{-1/2}/\ln\ell$. The different phases can thus be detected by the different asymptotic behaviour of Δ. This is in contrast to the universal asymptotic behaviour where for all coupling constants $\Delta \to a\ell^{-1/2}$ holds.

4.3.4. Numerical Results

Subsections 4.3.1 and 4.3.2 demonstrated the possibilities and freedom one possesses in setting up Flow Equations. In the following we will first restrain ourselves to the parameter regime $\epsilon = 0$ and $\delta = 0$ of the form-invariant Hamiltonian flow, since then the Flow Equations for the observable σ_z simplify considerably, see Eq. (4.92). We will then discuss the extended scheme.

We start by verifying the predictions of the universal asymptotic behaviour for the Ohmic bath, outlined in the last subsection. In contrast to the exactly solvable Dissipative Harmonic Oscillator, the constants a and ξ cannot be determined analytically. The self-consistent solution of the differential equations (4.111) and (4.119) yields the following values:

$$J_0 \approx 0.41 \quad , \quad a \approx 1.21 \quad , \quad \xi \approx 0.41$$

In Figure 4.3 the universal asymptotic functions $J(y)$ and $S(y)$ obtained from numerical integration of the Flow Equations are compared with the "analytic" solution following from the self-consistent evaluation of Eqs. (4.111) and (4.119). The asymptotic results do neither depend on the coupling strength α, nor on the explicit form of the cutoff function, nor on the value of ω_c.

The universal function $S(y)$ shows similar features as the normalized dynamic susceptibility for $\alpha = J_0/2 \approx 0.2$, shown in Figure 4 of Ref. [Cos96]. There, it was also noted that this function shows universal features, but a direct connection could not be established.

The symmetrized equilibrium correlation function $C(\omega)$ must of course depend on the initial conditions. Since the asymptotic functions $S(y)$ only differ by at most a constant for arbitrary initial conditions, this information must be contained in the primary and intermediate ℓ-range of the flow. This is characteristic for universal asymptotic behaviour and in contrast to non-universal asymptotic behaviour, where the intermediate time-scales of correlation functions are determined by the final ℓ-range of the flow. In Figure 4.4 the results of $C(\omega)$ for a Ohmic bath with sharp cutoff at $\omega_c = 30$ for different coupling strengths α are shown.

The spectral function $C(\omega)$ is obtained by integrating the Flow Equations of Eqs. (4.69) - (4.71) and (4.92) up to $\Delta^2\ell^* = 10^3$ where one is already in the asymptotic regime for the coupling strengths considered.[9] Notice that we do not employ a conservation law to build up the spectral functions, nor is our approach limited to small coupling strengths. But since the sum rule $h^2 + \sum_\alpha (\chi_\alpha^x)^2 = 1$ is *not* fulfilled, the final spectral function $C(\omega)$ does not fulfill the sum rule $\int_0^\infty d\omega C(\omega) = 1$ either. Independent from the cutoff parameter ω_c and bath type the sum rule only yields

[9] For higher coupling strengths one would have to integrate up to larger ℓ^*.

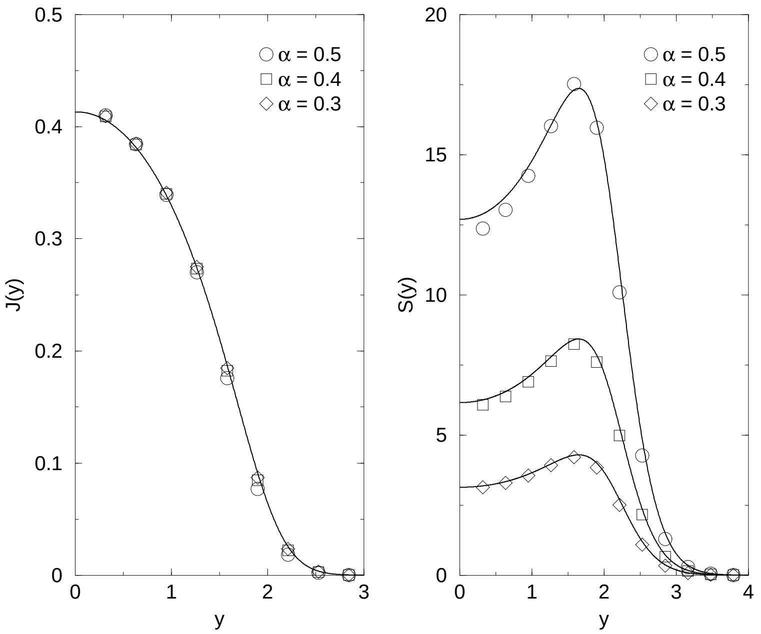

Figure 4.3.: The asymptotic spectral functions $J(y)$ and $S(y)$ obtained from the form-invariant flow for Ohmic coupling and $\epsilon = 0$ at $\Delta^2\ell^* = 10^3$ for different coupling constants α. The solid line resembles the "analytic" solution.

approximately 80 percent for small coupling constants ($\alpha \approx 0.1$) and $83 - 85$ percent for larger coupling constants.[10]

Nevertheless, $C(\omega)$ contains physical information. This is demonstrated in the inset of Figure 4.4 where the maximum of $C(\omega)$ is plotted for different cutoff frequencies ω_c as a function of the coupling strength α, according to the effective tunnel-matrix element Δ_{eff} of Eq. (4.33), following from the NIBA. One sees that the universal regime described by the NIBA is only reached for small coupling constants and for rather large ω_c.

We will now investigate the extended truncation scheme outlined in subsections 4.3.1 and 4.3.2. But we will restrain the operator flow to linear terms in the bosonic operators, i.e. $\psi^{\pm}_{\alpha,\alpha'} = 0$ and therefore also $\chi^e_\alpha = 0$ for all ℓ.

We will first specify the generator. The parameters of $\eta^{e,2}$ have already been chosen in subsection 4.3.1. The remaining parameters of the generator shall be fixed according to the canonical generator $\eta = [H_0, H]$. Still, we are free to choose the diagonal Hamiltonian as was pointed out in Chapter 3.

[10] Coupling strengths up to $\alpha = 2.5$ were tested.

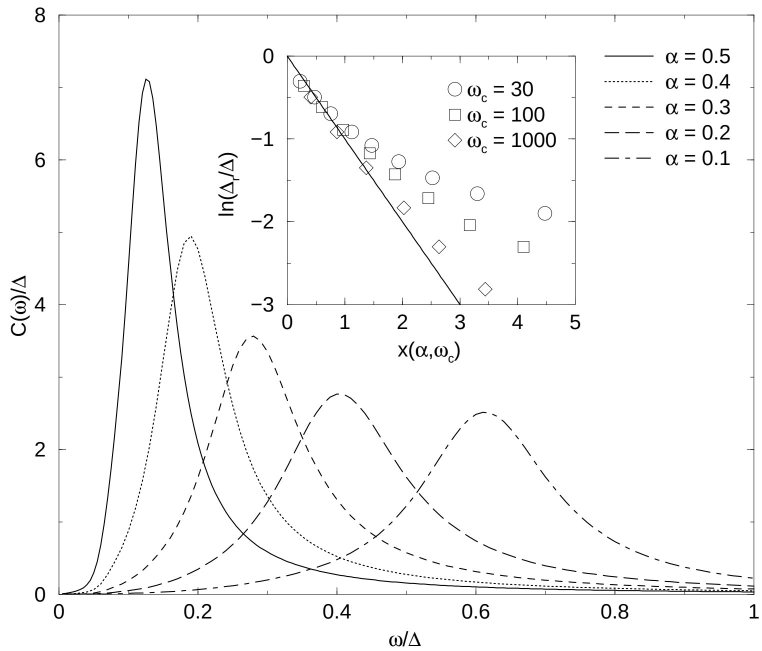

Figure 4.4.: The spectral functions $C(\omega)$ obtained from the form-invariant flow for Ohmic coupling $J(\omega) = 2\alpha\omega\Theta(\omega_c - \omega)$ with $\omega_c/\Delta = 30$ and $\epsilon = 0$ at $\Delta^2\ell^* = 10^3$ for different coupling constants α. Inset: Defining the maximum of $C(\omega)$ as Δ_r, $\ln(\Delta_r/\Delta)$ is plotted versus $x(\alpha,\omega_c) \equiv \alpha/(1-\alpha)\ln(\omega_c/\Delta) - \ln(\cos(\pi\alpha)\Gamma(1-2\alpha))/(2-2\alpha)$ for different cutoffs ω_c. The solid line resembles the NIBA result for Δ_{eff}.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \omega_\alpha b^\dagger_\alpha b_\alpha}$

One obvious choice is to set the diagonal Hamiltonian to be $H_0 = -\frac{\Delta}{2}\sigma_x + \omega_\alpha b^\dagger_\alpha b_\alpha$. This yields $\eta^y = \Delta\epsilon/2$, $\eta^e_\alpha = -\omega_\alpha\lambda^e_\alpha/2$, $\eta^x_\alpha = -\omega_\alpha\lambda^x_\alpha/2$, $\eta^y_\alpha = (\Delta\lambda^z_\alpha - \omega_\alpha\lambda^y_\alpha)/2$ and $\eta^z_\alpha = (-\omega_\alpha\lambda^z_\alpha + \Delta\lambda^y_\alpha)/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1a.

- $\boldsymbol{H_0 = \frac{\epsilon}{2}\sigma_z + \omega_\alpha b^\dagger_\alpha b_\alpha}$

Another choice for the diagonal Hamiltonian is given by $H_0 = \frac{\epsilon}{2}\sigma_z + \omega_\alpha b^\dagger_\alpha b_\alpha$. This yields $\eta^y = -\Delta\epsilon/2$, $\eta^e_\alpha = -\omega_\alpha\lambda^e_\alpha/2$, $\eta^x_\alpha = (-\omega_\alpha\lambda^x_\alpha + \epsilon\lambda^y_\alpha)/2$, $\eta^y_\alpha = (\epsilon\lambda^x_\alpha - \omega_\alpha\lambda^y_\alpha)/2$ and $\eta^z_\alpha = -\omega_\alpha\lambda^z_\alpha/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1b.

- $\boldsymbol{H_0 = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_\alpha b^\dagger_\alpha b_\alpha}$

Combining the previous choices we arrive at the diagonal Hamiltonian $H_0 = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_\alpha b^\dagger_\alpha b_\alpha$. Since the Pauli spin matrices do not commute,

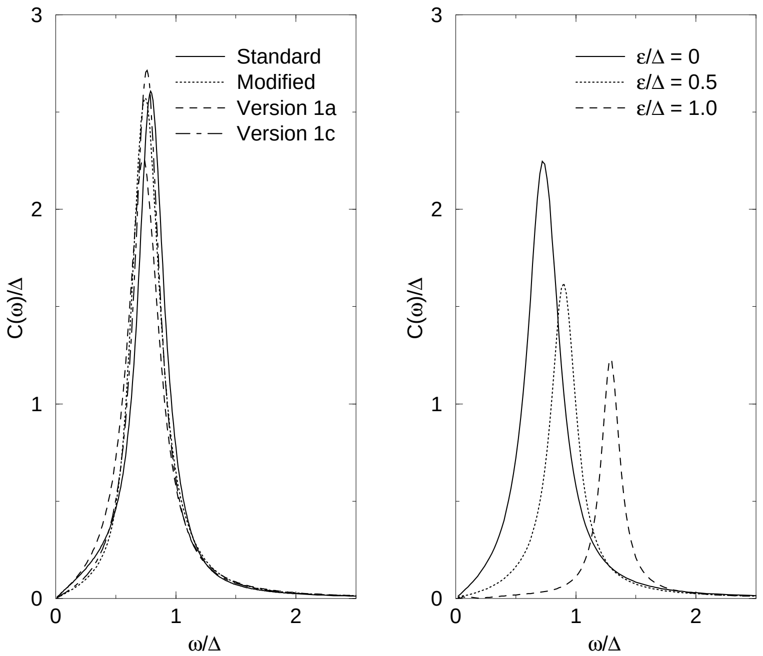

Figure 4.5.: The spectral function $C(\omega)$ for $J(\omega) = 2\alpha\omega\Theta(\omega_c - \omega)$ with $\alpha = 0.1$ and $\omega_c/\Delta = 10$. Left Hand Side: Employing the Standard and Modified Generator using the conservation law at $\Delta^2\ell^* = 10$, and the canonical generator of Versions 1a and 1c at $\Delta^2\ell^* = 10^6$ for zero bias $\epsilon = 0$. Right Hand Side: Employing the canonical generator of Version 1b at $\Delta^2\ell^* = 10^6$ for different bias ϵ.

we will first diagonalize the one-particle Hamiltonian $H_0^p = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z \to \frac{R}{2}\sigma_z$ with $R = \sqrt{\Delta^2 + \epsilon^2}$. The transformation induces different initial conditions for the Hamiltonian of Eq. (4.42) and for the initial observable. For the parameters of the canonical generator this yields $\eta^y = -\Delta R/2$, $\eta_\alpha^e = -\omega_\alpha\lambda_\alpha^e/2$, $\eta_\alpha^x = (-\omega_\alpha\lambda_\alpha^x + R\lambda_\alpha^y)/2$, $\eta_\alpha^y = (R\lambda_\alpha^x - \omega_\alpha\lambda_\alpha^y)/2$ and $\eta_\alpha^z = -\omega_\alpha\lambda_\alpha^z/2$. We will refer to the Flow Equations with this particular choice of the generator as Version 1c.

For Versions 1a and 1b the one-particle expectation values are determined according to the general scheme outlined in Chapter 3, i.e. the coupling terms are comprised in effective bosonic modes and the one-particle expectation values are evaluated with respect to the effective one-particle Hamiltonian. This yields $\langle\sigma_x\rangle = \Delta'/R'$ and $\langle\sigma_z\rangle = -\epsilon'/R'$ with $\Delta' \equiv \Delta + \frac{\lambda_\alpha^e\lambda_\alpha^x}{\omega_\alpha} - \frac{\lambda_\alpha^y\lambda_\alpha^z}{\omega_\alpha}$, $\epsilon' \equiv \epsilon - \frac{\lambda_\alpha^e\lambda_\alpha^z}{\omega_\alpha} - \frac{\lambda_\alpha^x\lambda_\alpha^y}{\omega_\alpha}$, and $R' \equiv \sqrt{\Delta'^2 + \epsilon'^2}$. For Version 1c the analogous expressions hold by replacing $\epsilon \to R$.

We want to comment on the asymptotic behaviour of the three versions. Version 1a exhibits non-universal asymptotic behaviour and yields a wrong long-time behaviour

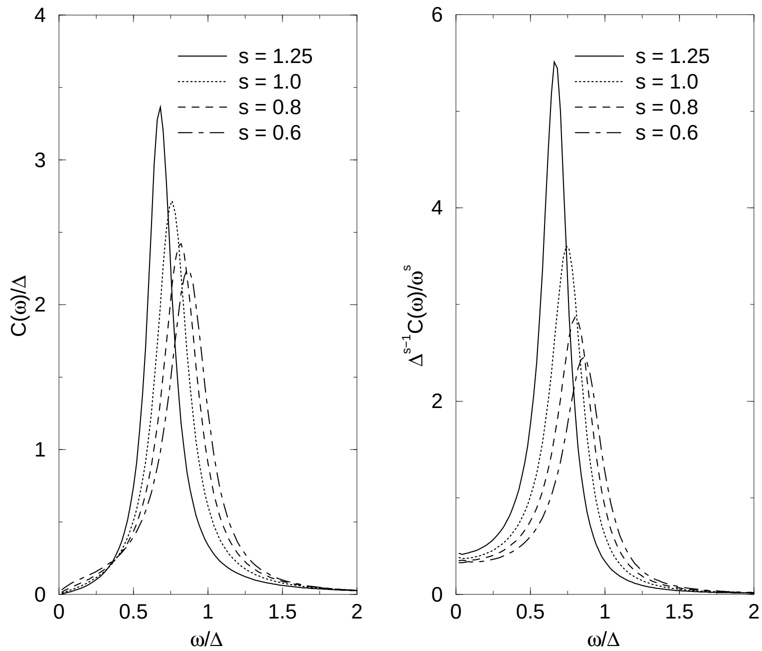

Figure 4.6.: The spectral function $C(\omega)$ (left hand side) and $C(\omega)/\omega^s$ (right hand side) for $J(\omega) = 2\alpha K^{1-s}\omega^s\Theta(\omega_c - \omega)$ with $\alpha = 0.1$, $\omega_c/\Delta = 10$, $K = 1$ and $\epsilon = 0$ at $\Delta\ell^* = 10^6$ for different bath types s, employing the canonical generator of Version 1c.

for finite bias $\epsilon \neq 0$. Version 2b exhibits non-universal asymptotic behaviour for zero bias $\epsilon = 0$ - but universal asymptotic behaviour for finite bias $\epsilon \neq 0$. Version 1c exhibits universal asymptotic behaviour within the entire parameter regime - also for sub- and super-Ohmic baths. In general, universal asymptotic behaviour, i.e. all system parameters tend to zero for $\ell \to \infty$, leads to more stable and reliable results.

The left hand side of Figure 4.5 displays various Flow Equation results for the symmetrized equilibrium correlation function $C(\omega)$ for a Ohmic bath with sharp cutoff at $\omega_c/\Delta = 10$ and coupling strength $\alpha = 0.1$ that were discussed in this chapter. The sum rule $\int d\omega C(\omega) = 1$ holds within 0.1 percent relative error for all versions - but differences are apparent. As was pointed out in Chapter 3, the sum rule does not provide a sufficient criterion for the quality of the Flow Equation results.

To contrast the results obtained from the different generators, we will again employ the Shiba relation given in Eq. (4.40). For Version 1a we obtain $\lim_{\omega\to 0} C(\omega)/\omega \approx 0.58$ and $2\alpha(2\chi_0)^2 \approx 0.46$, and Version 1b yields identical results within numerical errors. The best agreement is obtained for the canonical generator of Version 1c with $\lim_{\omega\to 0} C(\omega)/\omega \approx 0.37$ and $2\alpha(2\chi_0)^2 \approx 0.40$.

$C(\omega)$ of Version 1c almost coincides with $C(\omega)$ of the modified generator of subsection 4.2.2. The agreement with the NIBA result for intermediate time scales is even enhanced and practically one-to-one. Furthermore, the Flow Equations of Version 1c yield stable results for coupling constants up to $\alpha \approx 0.6$ where the sum rule still holds within 0.1 percent relative error and the Shiba relation is satisfied up to 25 percent relative error.

On the right hand side of Figure 4.5, $C(\omega)$ is shown for a Ohmic bath with sharp cutoff with $\omega_c/\Delta = 10$ and coupling strength $\alpha = 0.1$ for different bias ϵ. The results are obtained from the Flow Equations of Version 1b. For finite bias, the constant term $f^* \equiv f(\ell = \infty)$ is generated and yields $f^* \approx -0.55$ for $\epsilon/\Delta = 0.5$ and $f^* \approx -0.80$ for $\epsilon/\Delta = 1$. Since $\lambda_\alpha^i(\ell = \infty) = 0$ and $\lambda_\alpha^y(\ell = \infty) = 0$, we obtain $\langle\sigma_z\rangle = f^*$ which has to be compared with the free values $\langle\sigma_z\rangle \approx -0.45$ and $\langle\sigma_z\rangle \approx -0.71$ for $\epsilon/\Delta = 0.5$ and $\epsilon/\Delta = 1$ respectively.

Jointly with the constant contribution f^*, the sum rule of $C(\omega)$ is fulfilled within 7 percent relative error for $\epsilon/\Delta = 0.5$ and within 1 percent relative error for $\epsilon/\Delta = 1$. The maxima of $C(\omega)$ correspond to the weak coupling result $\Delta_b^* = \sqrt{\Delta^{*2} + \epsilon^2}$ within 3 percent relative error, Δ^* denoting the maximum of $C(\omega)$ in the un-bias case.

The left hand side of Figure 4.6 displays the Flow Equation results of $C(\omega)$ for the initial coupling function $J(\omega) = 2\alpha K^{1-s}\omega^s\Theta(\omega_c - \omega)$ with $\alpha = 0.1$, $K = 1$ and $\omega_c/\Delta = 10$ for different bath type parameters s, employing the canonical generator of Version 1c. The sum rule is fulfilled up to 0.01 percent relative error in all cases. The different long-time behaviour of the various bath types can be best seen on the right hand side of Figure 4.6, where $C(\omega)/\omega^s$ is plotted. For the super-Ohmic bath $s = 1.25$, the generalized Shiba relation holds approximately with $\lim_{\omega\to 0} C(\omega)/\omega^s \approx 0.42$ and $2\alpha(2\chi_0)^2 \approx 0.44$.

We want to mention that no constant term f is generated during the flow, including the bath types with $s = 0.8$ and $s = 0.6$. We thus observe *no* localization with respect to the above parameters for the sub-Ohmic baths. This in agreement with Refs. [Spo85] and [Keh96a] which predict a first order phase transition at some finite coupling strength for $s < 1$ - but in contradiction to the NIBA that states that there is always localization for sub-Ohmic baths and thus $\langle\sigma_z\rangle \neq 0$.[11]

In order to make explicit predictions on the crossover between coherent and incoherent tunneling and on the phase transition for the Ohmic and sub-Ohmic bath, two-boson processes might have to be included. Another improvement should be achieved by the sophistication of the evaluation of the one-particle expectation values which will also alter the bosonic normal ordering procedure. Suggestions were given in subsection 4.3.2. Moreover, the formulation of the Flow Equations with respect to a representation in which the reflection symmetry is spontaneously broken could prove to be preferable for larger coupling constants.

[11]The NIBA result might be due to ambiguous cutoff limits.

5. Brownian Motion in a Periodic Potential

In the previous chapter we considered the most fundamental dissipative quantum system. There the system exposed to dissipation was projected onto the two-dimensional Hilbert space. The general one-particle Hamiltonian is given by

$$H^p = \frac{\hat{p}^2}{2m} + V(\hat{q}) \quad . \tag{5.1}$$

In this chapter we want to consider a particle in a periodic potential, i.e. $V(\hat{q}) = V(\hat{q} + 2\pi q_0)$ with a period characterized by q_0.[1]

By this extension the virtue of the Flow Equation approach becomes apparent because the procedure of setting up and truncating the Flow Equations is easily transferred from the models considered in the previous chapters. We will basically follow the procedure that was used in the case of the Dissipative Harmonic Oscillator.

Again adopting the ideas of Caldeira and Leggett we assume the bath to be given by a set of non-interacting harmonic oscillators. But in contrary to their proposal to choose a *linear* coupling between the system and the environment we now choose the coupling to be *non-linear*. More precisely the coupling will be periodic in the position operator of the system with the same periodicity as the one-particle potential, i.e with period $2\pi q_0$. This will preserve the invariance of the entire Hamiltonian with respect to translations of multiples of $2\pi q_0$.

Intuitively one would assume that system properties should be independent of the specific realization of the coupling between system and bath. In fact it was shown that the Markovian master equations are universal if one models the coupling as a random matrix using random matrix theory [Lut99]. This confirms the intuition.

Another approach to motivate the periodic coupling ansatz is to describe a Josephson junction coupled to an electromagnetic field. It turns out that the coupling between the phase and the field is then described by a sine function [Zwe82].

[1]In the literature the unit circumference 2π is usually included in the definition of q_0.

5.1. General Flow Equations for the Hamiltonian

To describe a quantum mechanical Brownian particle in a periodic potential we shall start with the following Hamiltonian:

$$\begin{aligned}\hat{H} &= \frac{\hat{p}^2}{2m} - V_0 \sum_n v_n e^{in\hat{q}/q_0} \\ &+ \sum_\alpha \Big(\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{1}{2} m_\alpha \omega_\alpha^2 (\hat{x}_\alpha + \frac{\lambda_\alpha}{m_\alpha \omega_\alpha^2} q_0 \sum_n \kappa_n e^{in\hat{q}/q_0})^2 \Big)\end{aligned} \tag{5.2}$$

For H to be Hermitian there must hold $v_n = (v_{-n})^*$ and $\kappa_n = (\kappa_{-n})^*$. The operators are denoted by a hat which shall be dropped from now on. They obey the canonical commutation relations which read

$$[q, p] = i \quad , \quad [x_\alpha, p_{\alpha'}] = i\delta_{\alpha,\alpha'} \quad . \tag{5.3}$$

The generator η of the infinitesimal unitary transformations, which shall decouple the system from the bath for $\ell \to \infty$, shall be characterized by the constants η_α^q, η_α^p and $\eta_{\alpha,\alpha'}$ in the following way:

$$\begin{aligned}\eta &= i(q_0 \sin(q/q_0)\eta_\alpha^q p_\alpha + p\eta_\alpha^p x_\alpha + \eta_{\alpha,\alpha'} x_\alpha p_{\alpha'}) \\ &\equiv \eta^q + \eta^p + \eta_B\end{aligned} \tag{5.4}$$

Summation over the bath modes α is implied from now on. With respect to the general generator of the Dissipative Harmonic Oscillator of Eq. (2.67) the linear coupling q was replaced by the periodic coupling $q_0 \sin(q/q_0)$.[2] The Flow Equations thus preserve the periodicity of the initial Hamiltonian.

The commutator $[\eta, H]$ yields the following contributions:

$$\begin{aligned}[\eta^q, H] &= -(p\cos(q/q_0) + \cos(q/q_0)p)\eta_\alpha^q \frac{p_\alpha}{2m} \\ &+ q_0 \sin(q/q_0)\eta_\alpha^q m_\alpha \omega_\alpha^2 (x_\alpha + \frac{\lambda_\alpha}{m_\alpha\omega_\alpha^2} q_0 \kappa_n e^{inq/q_0})\end{aligned} \tag{5.5}$$

$$\begin{aligned}[\eta^p, H] &= -\frac{V_0}{q_0} v_n in e^{inq/q_0} \eta_\alpha^p x_\alpha - p\eta_\alpha^p \frac{p_\alpha}{m_\alpha} \\ &+ \eta_\alpha^p x_\alpha \lambda_{\alpha'} (x_{\alpha'} + \frac{\lambda_{\alpha'}}{m_{\alpha'}\omega_{\alpha'}^2} q_0 \kappa_n e^{inq/q_0}) \kappa_{n'} in' e^{in'q/q_0}\end{aligned} \tag{5.6}$$

$$[\eta_B, H] = -\eta_{\alpha,\alpha'} \frac{p_\alpha p_{\alpha'}}{m_\alpha} + \eta_{\alpha,\alpha'} x_\alpha m_{\alpha'} \omega_{\alpha'}^2 (x_{\alpha'} + \frac{\lambda_{\alpha'}}{m_{\alpha'}\omega_{\alpha'}^2} q_0 \kappa_n e^{inq/q_0}) \tag{5.7}$$

Summation over the Fourier modes n is implied from now on. The system parameters V_0, q_0 and m are invariant under the unitary transformation, i. e. independent of the

[2] More generally one could consider $\eta^q = iq_0 \sum_n \eta_{\alpha,n}^q e^{inq/q_0} p_\alpha$ with $\eta_{\alpha,n}^q = (\eta_{\alpha,-n}^q)^*$.

flow parameter ℓ. For the bath parameter ω_α we only obtain finite size effects which will be neglected.

In the following we want to consider the truncation scheme where the Hamiltonian of Eq. (5.2) remains form-invariant. We will therefore neglect the following normal ordered operators:

$$\mathcal{O}_1 = -\{p, : \cos(q/q_0) :\}\eta^q_\alpha \frac{p_\alpha}{2m} \tag{5.8}$$

$$\mathcal{O}_2 = \eta^p_\alpha \lambda_{\alpha'} \kappa_n in : e^{inq/q_0} : \bar{x}_\alpha \bar{x}_{\alpha'} : \tag{5.9}$$

The operator $\mathcal{O}_1$ is related to the operator proportional to σ_y neglected in the case of the Spin-Boson Model. Again the expectation value with respect to the free diagonal Hamiltonian vanishes.

In the above equations : ... : denotes normal ordering for system and bath operators respectively. The one-particle operators are normal ordered with respect to the ℓ-dependent one-particle Hamiltonian H^p. The bath operators are normal ordered with respect to

$$H_B = \frac{p_\alpha^2}{2m_\alpha} + \frac{1}{2} m_\alpha \omega_\alpha^2 (x_\alpha + \frac{\lambda_\alpha}{m_\alpha \omega_\alpha^2} q_0 \kappa_n \langle e^{inq/q_0} \rangle)^2 \quad . \tag{5.10}$$

We therefore introduced the shifted position operator $\bar{x}_\alpha \equiv x_\alpha + \delta_\alpha$ with $\delta_\alpha \equiv \frac{\lambda_\alpha}{m_\alpha \omega_\alpha^2} q_0 \kappa_n \langle e^{inq/q_0} \rangle$ in Eq. (5.9). With this truncation scheme we follow the procedure outlined in Chapter 3.

The parameters of the generator have to satisfy the following relations:

$$\begin{gathered}
\eta^q_\alpha \langle \cos(q/q_0) \rangle m_\alpha + \eta^p_\alpha m = 0 \\
\eta_{\alpha,\alpha'} m_{\alpha'} + \eta_{\alpha',\alpha} m_\alpha = 0 \\
\eta_{\alpha,\alpha'} m_{\alpha'} \omega_{\alpha'}^2 + \eta_{\alpha',\alpha} m_\alpha \omega_\alpha^2 - (\eta^p_\alpha \lambda_{\alpha'} + \eta^p_{\alpha'} \lambda_\alpha) \kappa_n in \langle e^{inq/q_0} \rangle = 0
\end{gathered} \tag{5.11}$$

Simplifying the notation by $\lambda_{\alpha,n} \equiv \lambda_\alpha \kappa_n$ the Flow Equations then read[3]

$$\begin{aligned}
\partial_\ell \tilde{v}_n &= i\sigma^{-1} \frac{1}{2} \eta^q_\alpha (\lambda_{\alpha,n-1} - \lambda_{\alpha,n+1}) - i\frac{n}{V_0} \eta^p_\alpha \lambda_{\alpha,n} \langle \bar{x}_\alpha^2 \rangle + i\frac{n}{V_0} \eta^p_\alpha \lambda_{\alpha',n} \delta_\alpha \delta_{\alpha'} \\
\partial_\ell \lambda_{\alpha,n} &= -\eta^q_\alpha m_\alpha \omega_\alpha^2 \frac{i}{2} n \delta_{|n|,1} - \eta^p_\alpha \sigma in \tilde{v}_n + \eta_{\alpha,\alpha'} \lambda_{\alpha',n} - i\frac{n\delta_{\alpha'}}{q_0} (\eta^p_\alpha \lambda_{\alpha',n} + \eta^p_{\alpha'} \lambda_{\alpha,n}) \quad ,
\end{aligned} \tag{5.12}$$

with $\sigma \equiv V_0/q_0^2$ and the renormalized potential

$$\tilde{v}_n \equiv v_n - \sigma^{-1} \frac{\lambda_{\alpha,n'} \lambda_{\alpha,n-n'}}{2m_\alpha \omega_\alpha^2} \quad . \tag{5.13}$$

[3]Notice that since on the left hand side of the Eqs. (5.12) there are n-depended quantities, summation over the Fourier modes on the right hand side is not implied.

The thermal expectation value of $\bar{x}_\alpha$ is taken over the free shifted bath of Eq. (5.10) and thus given by $\langle \bar{x}_\alpha^2 \rangle = (1+2n_\alpha)/(2m_\alpha\omega_\alpha)$ with $n_\alpha = (e^{\beta\omega_\alpha}-1)^{-1}$ and $\beta = 1/T$ the inverse temperature.

In order to write the Flow Equations in terms of $\tilde{v}_n$ one needed the relation

$$\sum_{n'} n'\kappa_{n'}\kappa_{n-n'} = \frac{n}{2}\sum_{n'}\kappa_{n'}\kappa_{n-n'} \quad . \tag{5.14}$$

The constants of the generator can be parameterized as follows:

$$\begin{aligned} \eta_\alpha^p &= \tilde{\lambda}_\alpha \langle \cos(q/q_0)\rangle f_\alpha/m \\ \eta_\alpha^q &= -\tilde{\lambda}_\alpha f_\alpha/m_\alpha \\ \eta_{\alpha,\alpha'} &= -\tilde{\lambda}_\alpha\tilde{\lambda}_{\alpha'}\langle\cos(q/q_0)\rangle(f_\alpha+f_{\alpha'})/(\omega_\alpha^2-\omega_{\alpha'}^2)/(m_{\alpha'}m) \quad , \end{aligned} \tag{5.15}$$

with $\tilde{\lambda}_\alpha \equiv -\sum_n \lambda_{\alpha,n}\langle ine^{inq/q_0}\rangle$.

A possible truncation scheme of order m is now given by considering all differential equations for $\tilde{v}_n$ with $n \leq m+1$ and the corresponding equations for $\lambda_{\alpha,n}$ with $n \leq m$.

In the following sections we will first consider a reflection-conserving periodic potential. Then there will be no bosonic shift, i.e. $\delta_\alpha = 0$ and we will be able to recover the known Flow Equations of the previous Chapters. A potential that explicitly breaks the reflection invariance will induce a non-zero shift in the bosonic modes, i.e. $\delta_\alpha \neq 0$. The general truncation scheme outlined above must then be applied. In the last section we will present a different approach to the quantum Brownian motion in a periodic potential where the bath is modeled by fermions.

5.2. Reflection-Conserving Periodic Potential

The Flow Equations preserve reflection symmetry, since the generator is invariant with respect to the parity operator. Thus starting with an even one-particle potential ($\mathrm{Im}v_n = 0$) and odd coupling functions ($\mathrm{Re}\kappa_n = 0$) the normal ordering with respect to the shifted modes reduces to the normal ordering with respect to the un-shifted modes, i.e. $\bar{x}_\alpha = x_\alpha$ or $\delta_\alpha = 0$. The Flow Equations reduce to

$$\begin{aligned} \partial_\ell \mathrm{Re}\tilde{v}_n &= -\sigma^{-1}\frac{1}{2}\eta_\alpha^q(\mathrm{Im}\lambda_{\alpha,n-1} - \mathrm{Im}\lambda_{\alpha,n+1}) + \frac{n}{V_0}\eta_\alpha^p \mathrm{Im}\lambda_{\alpha,n}\langle x_\alpha^2\rangle \\ \partial_\ell \mathrm{Im}\lambda_{\alpha,n} &= -\eta_\alpha^q m_\alpha\omega_\alpha^2\frac{1}{2}n\delta_{|n|,1} - \eta_\alpha^p\sigma n\mathrm{Re}\tilde{v}_n + \eta_{\alpha,\alpha'}\mathrm{Im}\lambda_{\alpha',n} \quad . \end{aligned} \tag{5.16}$$

In the following two subsections we will try to recover the previously discussed dissipative models embarking from the Flow Equations of Eq. (5.16). The Dissipative Harmonic Oscillator of Chapter 2 will be recovered in the limit $mq_0^2V_0 \gg 1$ involving all Fourier modes. The Spin-Boson Model of Chapter 4 will be recovered in the limit $mq_0^2V_0 \ll 1$ involving only one Fourier mode.

5.2.1. Recovering the Dissipative Harmonic Oscillator

Intuitively one expects to recover the Flow Equations of the Dissipative Harmonic Oscillator if one expands the cosine potential in a Taylor expansion and cuts the series after the quadratic term. It is thus useful to go back to position space via Fourier transformation

$$v(q) = -\sum_n v_n e^{inq/q_0} \quad , \quad \lambda_\alpha(q) = -\sum_n \lambda_{\alpha,n} e^{inq/q_0} \quad . \tag{5.17}$$

By this we take all Fourier modes of Eqs. (5.16) into account. We obtain the following coupled partial differential equations:

$$\partial_\ell \tilde{v}(q) = -\sigma^{-1} \sin(q/q_0) \eta_\alpha^q \lambda_\alpha(q) - \eta_\alpha^p q_0 \partial_q \lambda_\alpha(q) \langle x_\alpha^2 \rangle / V_0 \tag{5.18}$$
$$\partial_\ell \lambda_\alpha(q) = -\eta_\alpha^q m_\alpha \omega_\alpha^2 \sin(q/q_0) - \eta_\alpha^p \sigma q_0 \partial_q \tilde{v}(q) + \eta_{\alpha,\alpha'} \lambda_{\alpha'}(q) \tag{5.19}$$

Here $\tilde{v}(q) \equiv v(q) + \sigma^{-1} \frac{(\lambda_\alpha(q))^2}{2m_\alpha \omega_\alpha^2}$. Taylor expanding $\tilde{v}(q) \approx v^0 + \tilde{v}^2 (q/q_0)^2$ and $\lambda_\alpha(q) \approx \lambda_\alpha^1 (q/q_0)$ for $q \ll q_0$ then yields the following Flow Equations:

$$\partial_\ell \tilde{v}^2 = -\sigma^{-1} \eta_\alpha^q \lambda_\alpha^1 \quad , \quad \partial_\ell V_0 v^0 = -\eta_\alpha^p \lambda_\alpha^1 \langle x_\alpha^2 \rangle \tag{5.20}$$
$$\partial_\ell \lambda_\alpha^1 = -\eta_\alpha^q m_\alpha \omega_\alpha^2 - \eta_\alpha^p \sigma 2 \tilde{v}^2 + \eta_{\alpha,\alpha'} \lambda_{\alpha'}^1 \tag{5.21}$$

These are the Flow Equations of the Dissipative Harmonic Oscillator given in Eqs. (2.74) which still depend on η_α^p, η_α^q and $\eta_{\alpha,\alpha'}$. The only discrepancy now stems from the parameters of the generator themselves which for the periodic system are given in Eqs. (5.15).

With $\tilde{\lambda}_\alpha \approx \lambda_\alpha^1$ and with $\langle \cos(q/q_0) \rangle \approx 1$, equivalence is obtained. The first approximation follows within the limit $q \ll q_0$, the second approximation is justified if the on-site energy V_0 is large compared to the kinetic energy scale $1/(mq_0^2)$. Then we obtain for a harmonic potential $\langle \cos(q/q_0) \rangle = e^{-(32 m q_0^2 V_0 v^2)^{-1/2}} \approx 1$ for $m q_0^2 V_0 \gg 1$.

5.2.2. Recovering the Spin-Boson Model

Interpreting each well as a possible quantum state of the system one should obtain similar Flow Equations as those of the Spin-Boson Model. We thus consider the initial Hamiltonian of Eq. (5.2) with $v_1 \neq 0$, $\kappa_1 \neq 0$ and all other parameters zero and truncate the Flow Equations after one Fourier mode. This yields

$$\partial_\ell v_0 = \sigma^{-1} \eta_\alpha^q \mathrm{Im}\lambda_{\alpha,1} \quad , \quad \partial_\ell \mathrm{Re} v_1 = \eta_\alpha^p \mathrm{Im}\lambda_{\alpha,1} \langle x_\alpha^2 \rangle / V_0 \tag{5.22}$$
$$\partial_\ell \mathrm{Im}\lambda_{\alpha,1} = -\eta_\alpha^q m_\alpha \omega_\alpha^2 / 2 - \eta_\alpha^p \sigma \mathrm{Re} v_1 + \eta_{\alpha,\alpha'} \mathrm{Im}\lambda_{\alpha',1} \quad . \tag{5.23}$$

As in the Spin-Boson Model there is no potential renormalization, i.e. $\mathrm{Re}\tilde{v}_1 = \mathrm{Re} v_1$.

To make the connection to the Spin-Boson Model it is now preferable to change to the dual tight-binding representation of the Hamiltonian which was first noticed by

Schmid [Sch83]. The duality between the two models can also be formulated on the level of Hamiltonians [Sas96] which is the appropriate framework for our approach.

To establish the duality we have to replace the initial periodic coupling with the conventional linear coupling. This is not unproblematic since we initially introduced the periodic coupling in order to obtain an unambiguous decoupling scheme which would have not been the case if we had started directly from the tight-binding Hamiltonian. In Appendix E we present one possible truncation scheme which introduces another coupling term.

It will turn out that one has to renormalize the coupling constants in order to obtain the known result for the critical coupling α_c at which localization sets in. The replacement is then given by $2q_0 \sin(q/q_0)\mathrm{Im}\lambda_{\alpha,1} \approx \bar{\lambda}_\alpha q$ with $\bar{\lambda}_\alpha = \sqrt{2}\mathrm{Im}\lambda_{\alpha,1}/\pi$.

Let us briefly review the duality transformation outlined in Ref. [Sas96]. Performing the canonical transformation

$$\begin{aligned} p_\alpha \to -m_\alpha \omega_\alpha x_\alpha \quad &, \quad x_\alpha \to \frac{p_\alpha}{m_\alpha \omega_\alpha} + \frac{p}{\xi}\frac{\bar{\lambda}_\alpha}{m_\alpha \omega_\alpha^2} \quad , \\ q \to \frac{p}{\xi} \quad &, \quad p \to -\xi q + \sum_\alpha \frac{\bar{\lambda}_\alpha x_\alpha}{\omega_\alpha} \quad , \end{aligned} \tag{5.24}$$

with $\xi \equiv 1/q_0\tilde{q}_0$, $\tilde{q}_0$ being the tight-binding lattice spacing, the resulting Hamiltonian contains contributions which are bilinear in the bath position operators x_α and thus couples different modes. These terms can be formally transformed away to yield the tight-binding Hamiltonian:

$$H_{TB} = -V_0 \mathrm{Re} v_1 (e^{i\tilde{q}_0 p} + e^{-i\tilde{q}_0 p}) + \frac{\pi_\alpha^2}{2M_\alpha} + \frac{1}{2} M_\alpha \Omega_\alpha^2 (u_\alpha - \frac{d_\alpha}{M_\alpha \Omega_\alpha^2} q)^2 \quad , \tag{5.25}$$

where the new canonical operators π_α and u_α as well as the new bath parameters M_α and Ω_α were introduced. Further the relations $\xi\bar{\lambda}/(m_\alpha\omega_\alpha) = d_\alpha/(M_\alpha\Omega_\alpha)$ and $\xi^2/m = d_\alpha^2/(M_\alpha\Omega_\alpha^2)$ must hold.

The spectral function of the tight-binding model $J_{TB}(\omega) \equiv \pi d_\alpha^2/(2M_\alpha\Omega_\alpha)\delta(\omega-\omega_\alpha)$ is now related to the spectral function of the continuous model $J(\omega) \equiv \pi\bar{\lambda}_\alpha^2/(2m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha)$. For the Ohmic bath we obtain with $J(\omega) = \eta\omega$ the corresponding spectral function of the tight-binding model as $J_{TB}(\omega) = (\xi/\eta)^2\eta\omega/(1+(m\omega/\xi)^2)$.[4]

For an Ohmic bath, $\eta/\xi = 1$ and small mass m,[5] we can replace $J(\omega) \to J_{TB}(\omega)$. Further we can easily identify the tunnel matrix element $\Delta \equiv 2V_0\mathrm{Re}v_1$. We can thus deduce the Flow Equations for the transfer matrix element Δ and the spectral function $J_{TB}(\omega)$ from the Flow Equations of Eq. (5.16).

[4] Defining $J(\omega)$ without a high-frequency cutoff renders the initial Hamiltonian undefined but allows for a simple expression of $J_{TB}(\omega)$. Since the physics is determined by the low-energy behaviour of $J(\omega)$ this should not alter the physical picture.

[5] The mass m is only a parameter

The expectation value $c(\ell) \equiv \langle\cos(q/q_0)\rangle$ must now be calculated with respect to the corresponding tight-binding model. For this let $c_n^{(\dagger)}$ denote the creation and annihilation operators of the Wannier state at lattice site n so that $q = \tilde{q}_0 \sum_n n c_n^\dagger c_n$ and $e^{i\tilde{q}_0 p} = \sum_n c_n^\dagger c_{n+1}$. The expectation value of the cosine is then given by $c(\ell) \equiv \langle \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})\rangle/2$, where $\langle ... \rangle$ stands for the ground-state expectation value of

$$H^p = \frac{1}{2mq_0^2} \sum_n n^2 c_n^\dagger c_n - \frac{\Delta}{2} \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) \quad . \tag{5.26}$$

The one-particle Hamiltonian can also be obtained by performing the canonical dual transformation involving only the system operators, i.e. $q \to p/\xi$ and $p \to -\xi q$.

We are now able to explicitly set up the Flow Equations. Assuming the transfer matrix element Δ small compared to the on-site energy $1/(2mq_0^2)$ the expectation value yields $c(\ell) \approx 2mq_0^2\Delta$. Determining the parameters of the generator based on Eqs. (5.11) in the limit $mq_0^2 V_0 \ll 1$ yields $\eta_{\alpha,\alpha'} = 0$. A possible parameterization of η_α^q and η_α^p is then given by replacing $\tilde{\lambda}_\alpha$ from Eqs. (5.15) by $2\mathrm{Im}\lambda_{\alpha,1}$.

With $E_0 \equiv -V_0\tilde{v}_0$ we thus end up with the following Flow Equations:

$$\partial_\ell \Delta = 4\pi q_0^2 \Delta \int d\omega J(\omega,\ell) f(\omega,\ell)(1+2n(\omega)) \tag{5.27}$$

$$\partial_\ell E_0 = 2\pi q_0^2 \int d\omega J(\omega,\ell)\omega f(\omega,\ell) \tag{5.28}$$

$$\partial_\ell J(\omega,\ell) = 2J(\omega,\ell)(\omega^2 - 2\Delta^2) f(\omega,\ell) \tag{5.29}$$

Rescaling the tunnel-matrix element $\widetilde{\Delta} \equiv \sqrt{2}\Delta$ we arrive at the same Flow Equations as for the Spin-Boson Model of Eqs. (4.13) if we neglect the non-linear term in the differential equation for $J(\omega,\ell)$.

The localization scenario can now be observed by inserting $J(\omega,\ell)f(\omega,\ell) = \partial_\ell J(\omega,\ell)/(2(\omega^2 - \widetilde{\Delta}^2))$ into Eq. (5.27) and neglecting the ℓ-dependence of $\widetilde{\Delta}$ in the denominator. Replacing $\widetilde{\Delta}$ with its final value at $\ell = \infty$ yields the following self-consistency equation for $\widetilde{\Delta}_\infty \equiv \widetilde{\Delta}(\ell = \infty)$, see Ref. [Keh96a]:

$$\ln(\widetilde{\Delta}_\infty/\widetilde{\Delta}_0) = -2\pi q_0^2 \int d\omega \frac{J(\omega,0)}{\omega^2 - \widetilde{\Delta}_\infty^2} \tag{5.30}$$

Choosing $J(\omega,0) = \eta\omega\Theta(\omega_c - \omega)$ with η being the phenomenological friction parameter, we obtain the well-known scaling law of the renormalized tunnel-matrix element $\widetilde{\Delta}_\infty \propto \widetilde{\Delta}_0(\widetilde{\Delta}_0/\omega_c)^{\alpha/(1-\alpha)}$ with $\alpha \equiv \eta q_0'/(2\pi)$, where $q_0' \equiv 2\pi q_0$. In fact, recovering the correct expression of α as it was obtained in Refs. [Gui85] and [Fis85] fixed the renormalization condition of the coupling constants $\bar{\lambda}_\alpha$.

5.3. Reflection-Breaking Periodic Potential

We will now consider the situation where the one-particle potential is not invariant with respect to parity. This means that there is a distinguished direction. Transport phenomena are known from classical systems if a system with reflection-breaking periodic potential is exposed to correlated noise, see e.g. Ref. [Mie95]. Our objective is to describe these phenomena on the quantum level. Again we will approach the problem from two different perspectives, based on the Dissipative Harmonic Oscillator and on the Spin-Boson Model respectively.

5.3.1. Beyond the Dissipative Harmonic Oscillator

To set up the approximate Flow Equations we will again consider all Fourier components of Eqs. (5.12). Taylor expanding the renormalized potential and the coupling constants will in general also yield odd and even terms respectively, i.e. $\tilde{v}(q) \approx \tilde{v}^0 + \tilde{v}^1(q/q_0) + \tilde{v}^2(q/q_0)^2$ and $\lambda_\alpha(q) \approx \lambda_\alpha^0 + \lambda_\alpha^1(q/q_0)$ for $q \ll q_0$. This yields the following Flow Equations:

$$\partial_\ell \tilde{v}^1 = -\sigma^{-1}\eta_\alpha^q \lambda_\alpha^0 \quad , \quad \partial_\ell \tilde{v}^2 = -\sigma^{-1}\eta_\alpha^q \lambda_\alpha^1 \tag{5.31}$$

$$\partial_\ell V_0 \tilde{v}^0 = -\eta_\alpha^p \lambda_\alpha^1 \langle \bar{x}_\alpha^2 \rangle + \eta_\alpha^p \lambda_{\alpha'}^1 \delta_\alpha \delta_{\alpha'} \tag{5.32}$$

$$\partial_\ell \lambda_\alpha^0 = -\eta_\alpha^p \sigma 2\tilde{v}^1 + \eta_{\alpha,\alpha'} \lambda_{\alpha'}^0 - (\eta_\alpha^p \lambda_{\alpha'}^1 + \eta_{\alpha'}^p \lambda_\alpha^1)\delta_{\alpha'}/q_0 \tag{5.33}$$

$$\partial_\ell \lambda_\alpha^1 = -\eta_\alpha^q m_\alpha \omega_\alpha^2 - \eta_\alpha^p \sigma 2\tilde{v}^2 + \eta_{\alpha,\alpha'} \lambda_{\alpha'}^1 \tag{5.34}$$

Now the shift in the bath position operators x_α does not vanish, but yields $\delta_\alpha = -q_0\langle \lambda_\alpha(q)\rangle/(m_\alpha\omega_\alpha^2) \approx -(q_0\lambda_\alpha^0 + \langle q\rangle\lambda_\alpha^1)/(m_\alpha\omega_\alpha^2)$. The coupling parameters $\tilde{\lambda}_\alpha$ of Eqs. (5.15) are determined as $\tilde{\lambda}_\alpha \approx \lambda_\alpha^1$ for $q/q_0 \ll 1$. Evaluating the one-particle expectation values with respect to the tilted harmonic potential, we obtain $\langle q\rangle = -q_0 v^1/(2v^2)$ and $\langle \cos(q/q_0)\rangle = e^{-(32mq_0^2V_0v^2)^{-1/2}}\cos(\langle q\rangle/q_0)$.

5.3.2. Beyond the Spin-Boson Model

We will now try to consider as few Fourier modes of Eqs. 5.12 as possible. Since we want to describe a system in which the reflection symmetry is broken we need to keep track of at least two Fourier components of the one-particle potential.

Potential renormalization only occurs for the second Fourier component. Introducing the abbreviations $v_1^r \equiv \mathrm{Re}v_1$, $v_1^i \equiv \mathrm{Im}v_1^i$, $\tilde{v}_2^r \equiv \mathrm{Re}\tilde{v}_2$, $\tilde{v}_2^i \equiv \mathrm{Im}\tilde{v}_2^i$, $\lambda_\alpha^r \equiv \mathrm{Re}\lambda_{\alpha,1}$ and $\lambda_\alpha^i \equiv \mathrm{Im}\lambda_{\alpha,1}$, the truncated Flow Equations read:

$$\partial_\ell v_1^r = \eta_\alpha^p \lambda_\alpha^i \langle \bar{x}_\alpha^2\rangle/V_0 - \eta_\alpha^p \lambda_{\alpha'}^i \delta_\alpha \delta_{\alpha'}/V_0 \tag{5.35}$$

$$\partial_\ell v_1^i = -\eta_\alpha^p \lambda_\alpha^r \langle \bar{x}_\alpha^2\rangle/V_0 + \eta_\alpha^p \lambda_{\alpha'}^r \delta_\alpha \delta_{\alpha'}/V_0 \tag{5.36}$$

$$\partial_\ell \tilde{v}_2^r = -\sigma^{-1}\eta_\alpha^q \lambda_\alpha^i/2 \quad , \quad \partial_\ell \tilde{v}_2^i = \sigma^{-1}\eta_\alpha^q \lambda_\alpha^r/2 \tag{5.37}$$

$$\partial_\ell \lambda_\alpha^r = \eta_\alpha^p \sigma v_1^i + \eta_{\alpha,\alpha'}\lambda_{\alpha'}^r + \delta_{\alpha'}(\eta_\alpha^p \lambda_{\alpha'}^i + \eta_{\alpha'}^p \lambda_\alpha^i)/q_0 \tag{5.38}$$

$$\partial_\ell \lambda_\alpha^i = -\eta_\alpha^q m_\alpha \omega_\alpha^2 - \eta_\alpha^p \sigma \tilde{v}_1^r + \eta_{\alpha,\alpha'}\lambda_{\alpha'}^i - \delta_{\alpha'}(\eta_\alpha^p \lambda_{\alpha'}^r + \eta_{\alpha'}^p \lambda_\alpha^r)/q_0 \tag{5.39}$$

The flow of the energy shift is governed by $\partial_\ell V_0 \tilde{v}_0 = q_0^2 \eta_\alpha^q \lambda_\alpha^r$.

The only influence of the second Fourier mode on the above set of differential equations stems from the expectation values with respect to the one-particle system. Evaluating this expectation value perturbatively we will again change to the dual tight-binding representation. For this we have to again linearize the periodic coupling and the canonical transformation given in (5.24) needs to be extended since also an even coupling term is being generated during the flow. This yields

$$\begin{aligned} p_\alpha \to -m_\alpha \omega_\alpha x_\alpha \quad &, \quad x_\alpha \to \frac{p_\alpha}{m_\alpha \omega_\alpha} + \frac{p}{\xi} \frac{\bar{\lambda}_\alpha^i}{m_\alpha \omega_\alpha^2} - \frac{\bar{\lambda}_\alpha^r}{m_\alpha \omega_\alpha^2} \\ q \to \frac{p}{\xi} \quad &, \quad p \to -\xi q + \sum_\alpha \frac{\bar{\lambda}_\alpha^i x_\alpha}{\omega_\alpha} \quad . \end{aligned} \tag{5.40}$$

To obtain the duality between the continuous and the tight-binding representation, the procedure is now analogous to the one described in the previous subsection.

The one-particle expectation values are thus evaluated with respect to the tight-binding Hamiltonian $H^p = H_0 + V$ with $H_0 \equiv U \sum_n n^2 c_n^\dagger c_n$ and

$$V = -\frac{\Delta_1^c}{2} \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) - \frac{\Delta_2^c}{2} \sum_n (c_{n+2}^\dagger c_n + c_n^\dagger c_{n+2}) \tag{5.41}$$

$$- \frac{\Delta_1^s}{2i} \sum_n (c_{n+1}^\dagger c_n - c_n^\dagger c_{n+1}) - \frac{\Delta_2^s}{2i} \sum_n (c_{n+2}^\dagger c_n - c_n^\dagger c_{n+2}) \quad . \tag{5.42}$$

The transfer matrix elements yield $\Delta_n^c \equiv 2V_0 v_n^r$ and $\Delta_n^s \equiv 2V_0 v_n^i$ with $n = 1, 2$ and the on-site energy is given by $U = 2mq_0^2$.[6]

Let Δ denote the energy scale of the transfer matrix elements in the following. Evaluating the expectation value $\langle \cos(q/q_0) \rangle$ to first order in Δ/U does not involve the second Fourier mode. Effects coming from breaking the reflection symmetry can thus not be accounted for. When calculating the expectation value $\langle \cos(q/q_0) \rangle$ to second order in Δ/U, also the ground-state of H^p, denoted by $|\varphi\rangle_2$, has to be expanded to second order in Δ/U:

$$|\varphi\rangle_2 = |\varphi\rangle_0 + \frac{Q}{\epsilon_0 - H_0} V |\varphi\rangle_0 + \frac{Q}{\epsilon_0 - H_0} V \frac{Q}{\epsilon_0 - H_0} V |\varphi\rangle_0 \quad , \tag{5.43}$$

with $|\varphi\rangle_0 \equiv c_0^\dagger |0\rangle$, where $|0\rangle$ denotes the fermionic vacuum with $c_n |0\rangle = 0$ for all n. $Q \equiv 1 - |\varphi\rangle_{00}\langle\varphi|$ denotes the projection operator to make the series well-defined.

We thus obtain $c(\ell) \equiv \langle \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})/2 \rangle = \Delta_1^c/U + 3(\Delta_1^c \Delta_2^c + \Delta_1^s \Delta_2^s)/(4U^2)$ and $s(\ell) \equiv \langle \sum_n (c_{n+1}^\dagger c_n - c_n^\dagger c_{n+1})/(2i) \rangle = \Delta_1^s/U + 3(\Delta_1^c \Delta_2^s - \Delta_1^s \Delta_2^c)/(4U^2)$. The

[6] Notice that for the second Fourier component only the un-renormalized potential enters.

constant shift of the bosonic operators x_α is then given by $\delta_\alpha = q_0(2\lambda^r_\alpha c(\ell) - 2\lambda^i_\alpha s(\ell))/(m_\alpha\omega^2_\alpha)$.

Finally we need to determine the parameters of the generator. Since we are considering the one-particle expectation values up to second order in Δ/U, $\eta_{\alpha,\alpha'}$ does not vanish. Nevertheless we will use a different parameterization as given in Eqs. (5.15). With $\eta^p = c(\ell)2\lambda^i_\alpha f_\alpha/m$ and $\eta^p = -2\lambda^i_\alpha f_\alpha/m_\alpha$ we obtain

$$\eta_{\alpha,\alpha'} = -\frac{4}{m}\frac{(\lambda^i_\alpha\lambda^r_{\alpha'}f_\alpha + \lambda^i_{\alpha'}\lambda^r_\alpha f_\alpha)\Delta_1^{c2} + \lambda^i_\alpha\lambda^i_{\alpha'}(f_\alpha + f_{\alpha'})(\Delta^c_1\Delta^s_1)}{m_{\alpha'}(\omega^2_\alpha - \omega^2_{\alpha'})U^2} \quad . \tag{5.44}$$

This explicitly determines the Flow Equations of Eqs. (5.35) - (5.39).

5.4. Flow of Observables

To evaluate correlation functions we have to perform the same sequence of unitary transformations to the observables that led to the diagonalization of the Hamiltonian. Again, we will take advantage of the periodicity of the system and choose the ansatz that describes the flow of the position operator as

$$q(\ell) = q_0 h_n e^{inq/q_0} + \chi_{\alpha,n}e^{inq/q_0}\bar{x}_\alpha \quad , \tag{5.45}$$

with complex $h_n = (h_{-n})^*$ and $\chi_{\alpha,n} = (\chi_{\alpha,-n})^*$.

Under parity the position operator transforms like an odd function. Since the Flow Equations preserve the reflections symmetry we have Re$h_n = 0$ and Im$\chi_{\alpha,n} = 0$ for all n and ℓ if $\delta_\alpha = 0$. For $\delta_\alpha \neq 0$, this symmetry will be broken.

The commutator $[\eta, q]$ yields the following contributions:

$$[\eta, q_0 h_n e^{inq/q_0}] = inh_n\eta^p_\alpha e^{inq/q_0}\bar{x}_\alpha \tag{5.46}$$

$$\begin{aligned}[\eta, \chi_{\alpha,n}e^{inq/q_0}x_\alpha] = &-iq_0\eta^q_\alpha(\chi_{\alpha,n-1} - \chi_{\alpha,n+1})e^{inq/q_0}/2 \\ &+ in\eta^p_\alpha\chi_{\alpha',n}e^{inq/q_0}x_\alpha\bar{x}_{\alpha'}/q_0 + \eta_{\alpha,\alpha'}\chi_{\alpha',n}e^{inq/q_0}x_\alpha\end{aligned} \tag{5.47}$$

Neglecting normal ordered bosonic bilinears with respect to the shifted modes we obtain with $\partial_\ell q = [\eta, q]$ the following Flow Equations:

$$\begin{aligned}\partial_\ell h_n &= -i\eta^q_\alpha(\chi_{\alpha,n-1} - \chi_{\alpha,n+1})/2 + in\eta^p_\alpha\chi_{\alpha,n}\langle\bar{x}^2_\alpha\rangle/q_0^2 - \eta_{\alpha,\alpha'}\chi_{\alpha',n}\delta_\alpha/q_0 - \chi_{\alpha,n}\partial_\ell\delta_\alpha/q_0 \\ \partial_\ell\chi_{\alpha,n} &= inh_n\eta^p_\alpha + \eta_{\alpha,\alpha'}\chi_{\alpha',n} - in\eta^p_{\alpha'}\chi_{\alpha,n}\delta_{\alpha'}\end{aligned} \tag{5.48}$$

In the following we will again base our approximations on two limits - firstly considering all, and secondly only few Fourier modes. Like this we will be able to recover the known Flow Equations of the observables of the Dissipative Harmonic Oscillator and the Spin-Boson Model and also go beyond in a systematic manner.

5.4.1. On tracks of the Dissipative Harmonic Oscillator

In order to obtain the Flow Equations of the Dissipative Harmonic Oscillator we will consider all Fourier components and define the Fourier transforms as

$$h(q) = h_n e^{inq/q_0} \quad , \quad \chi_\alpha(q) = \chi_{\alpha,n} e^{inq/q_0} \quad . \tag{5.49}$$

The set of Flow Equations of (5.48) is thus given by the following coupled partial differential equations:

$$\begin{aligned} \partial_\ell h(q) &= \eta^q_\alpha \sin(q/q_0)\chi_\alpha(q) + \eta^p_\alpha \partial_q \chi_\alpha(q)\langle \bar{x}^2_\alpha\rangle/q_0 - \eta_{\alpha,\alpha'}\chi_{\alpha'}(q)\delta_\alpha/q_0 - \chi_\alpha(q)\partial_\ell\delta_\alpha/q_0 \\ \partial_\ell \chi_\alpha(q) &= q_0 \partial_q h(q)\eta^p_\alpha + \eta_{\alpha,\alpha'}\chi_{\alpha'}(q) - \eta^p_{\alpha'}\partial_q\chi_\alpha(q)\delta_{\alpha'} \quad . \end{aligned} \tag{5.50}$$

Expanding the q-dependent functions as $h(q) \approx h^0 + h^1 q/q_0$ and $\chi_\alpha(q) \approx \chi^0_\alpha$ for $q/q_0 \ll 1$ yields the initial conditions $h^1(\ell = 0) = 1$ and $\chi^0_\alpha(\ell = 0) = 0$. For $\delta_\alpha = 0$, the Flow Equations read

$$\partial_\ell h^1 = \eta^q_\alpha \chi^0_\alpha \quad , \quad \partial_\ell \chi^0_\alpha = h^1 \eta^p_\alpha + \eta_{\alpha,\alpha'}\chi^0_{\alpha'} \quad . \tag{5.51}$$

These are the same Flow Equations as given in Eqs. (2.86) and (2.87) when they still depend on the parameters of the generator. Thus making the same approximations that led to the equivalence of the Flow Equations of the Hamiltonian also yields equivalence in the case of the observable q.

If $\delta_\alpha \neq 0$, the constant term h^0 is being generated according to

$$\partial_\ell h^0 = -\eta_{\alpha,\alpha'}\chi^0_{\alpha'}\delta_\alpha/q_0 - \chi^0_\alpha \partial_\ell \delta_\alpha/q_0 \quad . \tag{5.52}$$

The odd reflection symmetry of the position operator is thus broken.

A measure for noise induced transport is $\langle q(t)\rangle$. Under the premise that $h^1 \to 0$, we obtain within the above ansatz $\langle q(t)\rangle = \langle q_0 h^0(\ell = \infty) + \chi^0_\alpha(\ell = \infty)\bar{x}_\alpha(t)\rangle$, where the average is taken with respect to $H(\ell = \infty)$. Since all coupling terms shall tend to zero for $\ell \to \infty$, there will be no time dependence of $\langle q(t)\rangle$. This is only achieved if one expands the Flow Equations (5.50) up to third order in q/q_0.

5.4.2. On tracks of the Spin-Boson Model

In order to obtain the Flow Equations of the Spin-Boson Model we will consider only one Fourier mode. Since we are interested in the evolution of the position operator given in the representation of Eq. (5.45), the initial condition of the parameters at $\ell = 0$ in Eq. (5.45) is then not unambiguous anymore. Following the procedure of subsection 5.2.2, where we replaced the periodic coupling $2q_0 \sin(q/q_0)$ by the renormalized linear coupling $\sqrt{2}q/\pi$, we obtain the initial conditions $h(\ell = 0) = -\pi/\sqrt{2}$ and $\chi_{\alpha,1} = 0$.

Choosing the parameters of the generator as in subsection 5.2.2, we obtain the following Flow Equations for a reflection-conserving periodic potential ($h^i \equiv -\sqrt{2}\mathrm{Im}h_1/\pi$, $\chi_\alpha^r \equiv \mathrm{Re}\chi_{\alpha,1}$, $\delta_\alpha = 0$):

$$\partial_\ell h^i = -2\Delta\bar{\lambda}_\alpha \chi_\alpha^r f_\alpha/(m_\alpha\omega_\alpha) \quad , \quad \partial_\ell \chi_\alpha^r = 2\pi^2 q_0^2 \Delta h^i \bar{\lambda}_\alpha f_\alpha \tag{5.53}$$

To make the connection to the differential equations that govern the flow of the z-component of the Pauli spin matrices σ_z, given in Eqs. (4.15), it is useful to introduce the spectral function $S(\omega,\ell) \equiv \sqrt{2}\bar{\lambda}_\alpha \mathrm{Re}\chi_{\alpha,1}/(2m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha)$. The Flow Equations then read

$$\partial_\ell h^i = \widetilde{\Delta}\int d\omega S(\omega,\ell) f(\omega,\ell) \tag{5.54}$$

$$\partial_\ell S(\omega,\ell) = -\widetilde{\Delta} h^i 2\pi q_0^2 J(\omega,\ell) f(\omega,\ell) + S(\omega,\ell)(\omega^2 - \widetilde{\Delta}^2) f(\omega,\ell) \quad . \tag{5.55}$$

Neglecting the two-boson processes in Eqs. (4.15), i.e. $\eta_{\alpha,\alpha'} = 0$, we obtain the same Flow Equations as in the case of the Spin-Boson Model, see Eqs. (4.16).

So far, we have succeeded in recovering the Flow Equations of the Spin-Boson Model for the observable, originating from the continuous model with a periodic potential. We now want to confirm that both approaches yield the same result for $\langle q^2 \rangle$, where $\langle ... \rangle$ stands for the ground-state expectation value with respect to the full Hamiltonian H of Eq. (5.2).

Let the weight of the system operator be completely transferred to the bath operators for $\ell \to \infty$, i.e. $h^i(\ell = \infty) = 0$. The expectation value is then given by $\langle q^2 \rangle = 2\langle \cos^2(q/q_0)\rangle (\chi_\alpha^r(\ell = \infty))^2/(m_\alpha\omega_\alpha)$. With the conservation law $(h^i)^2 + (\chi_\alpha^r)^2/(m_\alpha\omega_\alpha)/(\pi q_0)^2 = 1$ and $\langle \cos^2(q/q_0)\rangle \to \langle (\sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})/2)^2 \rangle \approx 1/2$ in leading order of $2mq_0^2\Delta$, we obtain $\langle q^2 \rangle = (q_0'/2)^2$ where $q_0' = 2\pi q_0$ denotes the distance between the wells.

For the Spin-Boson Model one trivially obtains $\langle q^2 \rangle = (q_0'/2)^2$ with $q = -q_0'\sigma_z/2$. This confirms that the initial condition $h(\ell = 0) = -\pi/\sqrt{2}$ leads to physically reasonable results.

We now turn to the Flow Equations of the position operator q in case of a reflection-breaking periodic potential. Considering only the first Fourier component the general Flow Equations are then given by

$$\begin{aligned}
\partial_\ell \mathrm{Re}h_1 &= -\eta_\alpha^p \mathrm{Im}\chi_{\alpha,1}\langle \bar{x}_\alpha^2\rangle/q_0^2 - \eta_{\alpha,\alpha'}\mathrm{Re}\chi_{\alpha',n}\delta_\alpha/q_0 - \mathrm{Re}\chi_{\alpha,n}\partial_\ell\delta_\alpha/q_0 \\
\partial_\ell \mathrm{Im}h_1 &= \eta_\alpha^p \mathrm{Re}\chi_{\alpha,1}\langle \bar{x}_\alpha^2\rangle/q_0^2 - \eta_{\alpha,\alpha'}\mathrm{Im}\chi_{\alpha',n}\delta_\alpha/q_0 - \mathrm{Im}\chi_{\alpha,n}\partial_\ell\delta_\alpha/q_0 \\
\partial_\ell \mathrm{Re}\chi_{\alpha,1} &= -\mathrm{Im}h_1\eta_\alpha^p + \eta_{\alpha,\alpha'}\mathrm{Re}\chi_{\alpha',1} + \eta_{\alpha'}^p \mathrm{Im}\chi_{\alpha,1}\delta_{\alpha'} \\
\partial_\ell \mathrm{Im}\chi_{\alpha,1} &= \mathrm{Re}h_1\eta_\alpha^p + \eta_{\alpha,\alpha'}\mathrm{Im}\chi_{\alpha',1} - \eta_{\alpha'}^p \mathrm{Re}\chi_{\alpha,1}\delta_{\alpha'} \quad .
\end{aligned} \tag{5.56}$$

Again terms are generated during the flow which do not transform like an odd function. This is due to the different normal ordering procedure, i.e. $\delta_\alpha \neq 0$.

A measure for noise induced transport shall again be given by $\langle q(t)\rangle$. Under the premise that $\mathrm{Im}h_1 \to 0$ for $\ell \to \infty$ and performing the duality transformation $\cos(q/q_0) \to \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})/2$ and $\sin(q/q_0) \to \sum_n (c_{n+1}^\dagger c_n - c_n^\dagger c_{n+1})/(2i)$, we obtain:

$$\langle q(t)\rangle = \langle \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})(t)\rangle (q_0 \mathrm{Re}h_1(\ell=\infty) + \chi_{\alpha,1}(\ell=\infty)\langle \bar{x}_\alpha(t)\rangle) \tag{5.57}$$

The average is taken with respect to $H(\ell=\infty)$. With $\lambda_\alpha^i(\ell=\infty)=0$ and $\lambda_\alpha^{r\,*} \equiv \lambda_\alpha^r(\ell=\infty)$ we obtain

$$H(\ell=\infty) = H^p(\ell=\infty) + \omega_\alpha(b_\alpha^\dagger + \lambda_\alpha^{r\,*}/(2\omega_\alpha))(b_\alpha + \lambda_\alpha^{r\,*}/(2\omega_\alpha)) + E^* \quad . \tag{5.58}$$

If either $\mathrm{Re}h_1(\ell=\infty) \neq 0$ or $\lambda_\alpha^{r\,*} \neq 0$, the expectation value of Eq. (5.57) yields a finite result since $\delta_\alpha(\ell=\infty) = q_0 2\lambda_\alpha^{r\,*} c(\ell=\infty)$. Further, we have $v_2(\ell=\infty) \neq 0$ or equivalently $\Delta_2^{c/s}(\ell=\infty) \neq 0$. This indicates noise induced transport since $\langle q(t)\rangle$ is then finite and time-dependent.

5.5. Tomonaga-Luttinger Model with Impurity

In the last section we will choose a different approach to the problem of Brownian motion in a periodic potential with Ohmic dissipation. It is based on the fact that the model is related to the Tomonaga-Luttinger Model (TL model) with an impurity, see e.g. the book of Weiss [Wei99]. The role of the coupling constant α is then taken by $v = \lim_{q\to 0} v_q$, where v_q is the Fourier transform of the two-body potential. The critical coupling strength $\alpha_c = 1$ corresponds to non-interacting electrons $v = 0$, the localized regime is resembled by repulsive electron-electron interaction, i.e. $v > 0$.

This opens up a new approach to the localization phenomena since the approximation scheme outlined in Section 2.2 is suitable for small interactions. The "exactly solvable point", which is the non-interacting fermion system and around which we are expanding the Flow Equations, thus lies just at the phase separation point.

To describe the transport properties of a particle in a cosine potential coupled to an Ohmic bath the initial Hamiltonian shall now be given by

$$H \equiv H_0 + H_{ee} + H_i = \sum_{q\neq 0} \omega_q^0 b_q^\dagger b_q + \sum_{q\neq 0} v_q^0 (b_q b_{-q} + b_{-q}^\dagger b_q^\dagger) + \lambda \psi^\dagger \psi \quad , \tag{5.59}$$

where the impurity is located at $x = 0$. The bosonic operators $b_q^{(\dagger)}$ with wave numbers $q = 2\pi n/L$, $n \in \mathbb{Z}$ obey the canonical commutation relations $[b_q, b_{q'}^\dagger] = \delta_{q,q'}$ and the initial conditions are given by $\omega_q^0 = v_F|q|(1 + v_q/2\pi v_F)$ and $v_q^0 = |q|v_q/4\pi$, where v_F denotes the Fermi velocity and v_q is the Fourier transform of the electron-electron interaction. For details see section 2.2.

The operator $\psi \equiv \psi(x = 0)$ denotes the fermionic field operator at $x = 0$. They obey the canonical anti-commutation relations. The impurity strength is given by λ and corresponds to the amplitude of the cosine potential.

The impurity term H_i is usually split into two contributions, i.e. a forward scattering and a backward scattering part. With $\psi \equiv \psi_L + \psi_R$ they read

$$H_i = \lambda^F(\psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L) + \lambda^B(\psi_R^\dagger \psi_L + \psi_L^\dagger \psi_R) \equiv H_F + H_B \quad . \tag{5.60}$$

The fermionic fields of the left- and right-movers are related to the fermionic ladder operators in the usual way, i.e. $\psi_{L/R} \equiv \sum_k c_k^{L/R}$, where $c_k^{L/R}$ obey the canonical anti-commutation relation $\{c_k^i, c_{k'}^{i'\,\dagger}\} = \delta_{i,i'}\delta_{k,k'}$ with $i, i' = L, R$. Expressing also the bosonic operators in fermionic ladder operators leads to the following commutation relation:

$$[b_q^{(\dagger)}, \psi_{L/R}] = -\Theta(\mp q) n_q^{-1/2} \psi_{L/R} \quad , \tag{5.61}$$

where $n_q \equiv |q|L/(2\pi) \in \mathbb{N}$, see section 2.2.

The forward scattering term can be expressed by the bosonic density fluctuations, i.e. $H^F = \sum_{q\neq 0} n_q^{1/2} L^{-1} \lambda_q^F (b_q + b_q^\dagger)$, where we neglected the term proportional to the number-of-particle operator of the left- and right-movers. This is an indication that the backscattering term will dominated the physical behaviour of the system. The initial conditions are given by $\lambda_q^F(\ell=0)=\lambda$ and $\lambda^B(\ell=0)=\lambda$.

The generator of the infinitesimal transformations shall consist of three parts $\eta \equiv \eta^{ee}+\eta^F+\eta^B$ according to the canonical generator with generalized parameters to be determined later:

$$\eta^{ee} = \sum_{q\neq 0} \eta_q^{ee}(b_q b_{-q} - b_{-q}^\dagger b_q^\dagger) \quad , \quad \eta^F = \sum_{q\neq 0} \eta_q^F (b_q - b_q^\dagger) \quad , \tag{5.62}$$

$$\eta^B = \sum_{q\neq 0} \eta_q^B ((b_q^\dagger \psi_R^\dagger \psi_L + \psi_R^\dagger \psi_L b_q) - h.c.) \quad . \tag{5.63}$$

The operator structure in η^B will appear frequently. For abbreviational purposes we will therefore define $\Psi_q \equiv b_q^\dagger \psi_R^\dagger \psi_L - \psi_R^\dagger \psi_L b_q$.[7]
The commutator $[\eta^{ee}, H]$ yields the following contributions:

$$[\eta^{ee}, H_0] = \sum_{q\neq 0} \omega_q(\eta_q^{ee}+\eta_{-q}^{ee})(b_q b_{-q} + b_{-q}^\dagger b_q^\dagger) \tag{5.64}$$

$$[\eta^{ee}, H_{ee}] = \sum_{q\neq 0} (\eta_q^{ee}+\eta_{-q}^{ee})(v_q+v_{-q})(b_q b_q^\dagger + b_q^\dagger b_q) \tag{5.65}$$

$$[\eta^{ee}, H_F] = \sum_{q\neq 0} n_q^{-1/2} L^{-1} (\eta_q^{ee}+\eta_{-q}^{ee})\lambda_{-q}^F (b_q + b_q^\dagger) \tag{5.66}$$

$$\begin{aligned} [\eta^{ee}, H_B] &= \sum_{q\neq 0} (\eta_q^{ee}+\eta_{-q}^{ee})\lambda^B \mathrm{sgn}(q) n_q^{-1/2} (\Psi_q + h.c.) \\ &- \sum_{q\neq 0} \eta_q^{ee} \lambda^B 2 n_q^{-1} (\psi_R^\dagger \psi_L + h.c.) \end{aligned} \tag{5.67}$$

The commutator $[\eta^F, H]$ yields the following contributions:

$$[\eta^F, H_0] = \sum_{q\neq 0} \eta_q^F \omega_q (b_q + b_q^\dagger) \quad , \quad [\eta^F, H_{ee}] = \sum_{q\neq 0} \eta_q^F (v_q + v_{-q})(b_q + b_q^\dagger) \tag{5.68}$$

$$[\eta^F, H_F] = \sum_{q\neq 0} n_q^{-1/2} L^{-1} 2 \eta_q^F \lambda_q^F \tag{5.69}$$

[7]Notice the different sign.

The commutator $[\eta^B, H]$ yields the following contributions:

$$[\eta^B, H_0] \approx -\sum_{q\neq 0} \eta_q^B \omega_q (\Psi_q + h.c.) \tag{5.70}$$

$$[\eta^B, H_{ee}] \approx \sum_{q\neq 0} \eta_{-q}^B (v_q + v_{-q})(\Psi_q + h.c.) + \sum_{q\neq 0} \eta_q^B (v_q + v_{-q}) \mathrm{sgn}(q) n_q^{-1/2} 2(\psi_R^\dagger \psi_L + h.c.) \tag{5.71}$$

$$\begin{aligned}[\eta^B, H_B] = &-\sum_{q\neq 0} \eta_q^B \lambda^B \mathrm{sgn}(q) n_q^{-1/2} \big((4\psi_R^\dagger \psi_R \psi_L^\dagger \psi_L + k_F/\pi(\psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L)) + h.c.\big) \\ &+ k_F/\pi \sum_{q\neq 0} \eta_q^B \lambda^B (b_q^\dagger (\psi_R^\dagger \psi_R - \psi_L^\dagger \psi_L) + h.c)\end{aligned} \tag{5.72}$$

The symbol $\approx$ in Eqs. (5.70) and (5.71) signifies that we only consider operators that contain less or equal than four fermionic operators of the left- and right-movers $c_k^{L/R(\dagger)}$. This is our truncation scheme which should be valid for small electron-electron interaction v_q, see Section 2.2. Moreover the neglected terms yield a vanishing ground-state expectation value with respect to the free bosonic bath.

In Eq. (5.72) there appears the factor k_F/π. It emerges from the regularization of the anti-commutation relation $\{\psi_{L/R}, \psi_{L/R}^\dagger\} = L^{-1}\sum_k \approx N/L$, having the restriction of the sum to the first Brillioun zone in mind.

We will now look more closely at Eq. (5.72). The term that contains four fermionic field operators $\psi_{L/R}^{(\dagger)}$ can again be expressed through bosonic density fluctuations. It couples only left-movers with right-movers and therefore corresponds to the g_1-processes in the g-ology notation of Ref. [Sol79]. But since the translational symmetry is broken by the impurity, momentum conservation does not hold anymore.

The last term will generate a new interaction term between the bosonic density fluctuations that couples different momenta also of the same branch, i.e. left-movers to left-movers and right-movers to right-movers. The general term that is being generated by the Flow Equations thus reads $H_R \equiv L^{-1}\sum_{q,q'\neq 0}(R_{q,q'}^1 b_q^\dagger b_{q'} + R_{q,q'}^2 (b_q b_{q'} + b_{q'}^\dagger b_q^\dagger))$.

This contribution had to be included into the flow of the Hamiltonian which would complicate the Flow Equations. There is evidence based on investigations of the Tomonaga-Luttinger Model with open boundaries that these terms do not alter the universal features of the model [Med00]. We will therefore neglect these new interaction terms.

We will now specify the flow. The generators η^{ee} and η^F are chosen according to the canonical generator $\eta^c \equiv [H_0, H]$. This yields $\eta_q^{ee} = -\omega_q(v_q + v_{-q})$ and $\eta_q^F = -\omega_q n_q^{1/2} L^{-1} \lambda_q^F$. The generator η^B is chosen in order to eliminate the newly generated terms that contain the operator $(\Psi_q + h.c.)$. This yields

$$\eta_q^B = \mathrm{sgn}(q) n_q^{-1/2} \lambda^B \frac{(\eta_q^{ee} + \eta_{-q}^{ee})}{\omega_q + (v_q + v_{-q})} \quad . \tag{5.73}$$

We are now ready to set up the explicit Flow Equations from $\partial_\ell H = [\eta, H]$. With $\omega_q = \omega_{-q}$ and $v_q = v_{-q}$, the Flow Equations for the bulk parameters read

$$\partial_\ell \omega_q = -16\omega_q v_q^2 \quad , \quad \partial_\ell v_q = -4\omega_q^2 v_q \quad . \tag{5.74}$$

These are the same Flow Equations as in the case without the impurity. The solution is thus given by Eqs. (2.42) and (2.43). The asymptotic behaviour of the coupling $v_q(\ell)$ turns out to be crucial for the following calculations. It can be deduced from the exact solution and yields $v_q(\ell) \to v_q^0(\tilde{\omega}_q/\omega_q^0)e^{-4\tilde{\omega}_q^2\ell}$ for $\ell \to \infty$.

The Flow Equations for the forward and backward scattering terms read:

$$\partial_\ell \lambda_q^F = -\lambda_q^F(\omega_q^2 + 6\omega_q v_q) + 2(\lambda^B)^2 \sum_{q'>0} n_{q'}^{-1} \frac{8\omega_{q'} v_{q'}}{\omega_{q'} + 2v_{q'}} \tag{5.75}$$

$$\partial_\ell \lambda^B = \lambda^B \sum_{q>0} \frac{8\omega_q v_q}{n_q} \frac{(\omega_q - 2v_q)^2}{\tilde{\omega}_q^2} \tag{5.76}$$

We discern that the flow of the impurity strength delicately depends on the sign of the interaction potential v_q. For attractive potentials $v_q < 0$ the impurity strength λ^B decreases, for repulsive potentials $v_q > 0$ the impurity strength λ^B increases.

We will now show that for attractive electron-electron interactions λ^B tends to zero and that for repulsive electron-electron interaction λ^B consequently tends to infinity. We will thus recover the result of Kane and Fisher based on a one-loop renormalization group analysis that in the case of repulsive fermions an arbitrarily small impurity potential cuts the one-dimensional chain in two distinct parts.

Eq. (5.76) is easily integrated and yields $\lambda^B(\ell) = \lambda^B(\ell = 0)\exp(\int_0^\ell d\ell' S(\ell'))$, where we defined

$$S \equiv \sum_{q>0} \frac{8\omega_q v_q}{n_q} \frac{(\omega_q - 2v_q)^2}{\tilde{\omega}_q^2} \to \sum_{q>0} \frac{v_q^0}{n_q} \frac{\tilde{\omega}_q^2}{\omega_q^0} e^{-4\tilde{\omega}_q^2\ell} \tag{5.77}$$

and the limit was taken for $\ell \to \infty$.

If we choose the interaction potential as a step function with momentum cutoff q_c, i.e. $v_q^0 = v\Theta(q_c - |q|)$, then the sum can be performed analytically in the thermodynamic limit $L \to \infty$ and $N/L = \text{const.}$:

$$S \to 8\tilde{\omega}^2 \frac{v}{\omega} \int_0^{q_c} dq q e^{-4\tilde{\omega}_q^2\ell} = \frac{v}{\omega}\ell^{-1}(1 - e^{-4\tilde{\omega}_{q_c}^2\ell}), \tag{5.78}$$

where we defined $\tilde{\omega} \equiv \lim_{q\to 0} \tilde{\omega}_q/q$ and $\omega \equiv \lim_{q\to 0} \omega_q^0/q$. For a general potential with $\partial_q^2 v_q|_{q=0} = 0$ one obtains the same generic result for $\ell \to \infty$ within a saddle point expansion. The asymptotic behaviour of the backscattering impurity potential is thus given by $\lambda^B \to \ell^{v/\omega}$, which leads to the scenario described above.

What is now left is to verify that the forward scattering potential λ_q^F will be negligible compared to λ_q^B for $\ell \to \infty$. We will first determine the asymptotic behaviour of the inhomogeneous part of Eq. (5.75). For this we have to evaluate the sum over q:

$$\sum_{q>0} n_q^{-1} \frac{8\omega_q v_q}{\omega_q + 2v_q} \to 8\tilde{\omega}\frac{v}{\omega}\int_0^{q_c} dq e^{-4\tilde{\omega}_q^2 \ell} = 2\pi^{1/2}\frac{v}{\omega}\ell^{-1/2}\mathrm{erf}(2\tilde{\omega}_{q_c}\sqrt{\ell}) \quad , \tag{5.79}$$

with the error function $\mathrm{erf}(x) \equiv 2\pi^{-1/2}\int_0^x dx' e^{-x'^2} \to 1 - e^{-x^2}/(x\pi)$ for $x \to \infty$.

The differential equation of (5.75) can thus be solved for $\ell \to \infty$. The leading term is given by $\lambda_q^F = 2\pi^{1/2}(v/\omega)(\lambda_*^B/\tilde{\omega}_q)^2 \ell^{2v/\omega - 1/2}$, where λ_*^B denotes the ℓ-independent asymptotic part of λ^B.

Since $2v/\omega = v/(2\pi v_F + v)$ we see that the forward scattering impurity strength tends to zero for $v \le 2\pi v_F$. For $v > 2\pi v_F$ and repulsive interaction it goes to infinity for $\ell \to \infty$ but with a lower power-law behaviour than the backward scattering impurity coupling. It will therefore always resemble the less relevant contribution to the asymptotic flow.[8]

[8] Of course one must question if the Flow Equations still hold for $v > 2\pi v_F$ since the approximations should only be justified for small interaction coupling v_q.

6. Summary and Outlook

Throughout this work, dissipative quantum systems were investigated by means of Flow Equations. Our interest was twofold: Firstly, we wanted to improve and generalize the rather new method of Flow Equations; secondly, we wanted to obtain new results in the rather old research topic of dissipative quantum systems.

To set up Flow Equations for dissipative systems and to evaluate equilibrium correlation functions, we mainly followed the approach outlined in Ref. [Keh97]. There, the initial Hamiltonian was given in the usual representation of the Caldeira-Leggett Model. During the observable flow, initial fermionic operators were transformed into a series of bosonic ladder operators. To strengthen this approach it was shown in subsection 2.1 that the infinite series yielded consistent and exact results.

In Chapter 3, a numerically solvable model was considered. A general truncation scheme was established that produced excellent results compared with the numerical solution. But it was also pointed out that a general scheme for the operator flow was missing. More explicitly, truncation of the series of the observable flow after the linear or bilinear terms did not yield satisfactory results for the entire parameter regime as - especially close to resonances - even high orders of the series expansion carried considerable weight.

In Chapter 4, Flow Equations for the Spin-Boson Model with broken reflection symmetry were established. In contrast to the symmetric model, the flow of the operator was then not confined to a subspace - but all possible operators within the truncation scheme were generated. This also gave rise to a constant contribution in the expansion of the x- and z-component of the Pauli spin matrices which was related to their expectation values as $\ell \to \infty$. New numerical results for equilibrium correlation functions covering a wide range of the parameter space including the bath type were presented.

Finally, Quantum Brownian Motion in a Periodic Potential was investigated. Departing from this general model, the Flow Equations of the Dissipative Harmonic Oscillator and of the Spin-Boson Model were recovered. Further, Flow Equations for a reflection-breaking periodic potential were set up, employing the previously developed procedures. Evidence for noise induced transport was established.

A general aspect of this work was the observation of universal asymptotic behaviour. There, all system parameters of the initial Hamiltonian tended to zero, governed by an universal asymptotic decay. The asymptotic spectral function of the coupling constants was described by a universal function of the composite variable $y = \omega\sqrt{\ell}$, depending on neither initial condition - but the bath type. The same held for the spectral function characterizing the observable flow. From this, the correct long-time behaviour of dynamic equilibrium correlation functions for the Dissipative Harmonic Oscillator could be derived. Furthermore, Flow Equations which exhibited universal asymptotic behaviour yielded more stable and reliable numerical results.

The topic of dissipative quantum systems was also addressed from a different perspective whereby the bath was not resembled by bosons - but by fermions. As a first step, Flow Equations were applied to the Tomonaga-Luttinger Model. By employing the bosonic representation of the fermionic field operator, the exact correlation functions were recovered. Using the standard fermionic representation, the Flow Equation approach yielded the generic algebraic behaviour of correlation functions close to the Fermi surface - but only in the limit of small interaction strengths. Nevertheless, the *exact* anomalous dimension was recovered.

In Chapter 5, an impurity was added to the Tomonaga-Luttinger liquid and the result of Kane and Fisher was confirmed such that in the asymptotic regime the backward scattering impurity strength tended to infinity (zero) for repulsive (attractive) electron-electron interaction.

Of course, a few points were left open. Arguably the most crucial one is the lack of a controlled scheme for the operator flow. One possibility to cure this short-come could be to couple the flow of the Hamiltonian and of the observable through an auxiliary operator. The extended Flow Equations would thus read

$$\partial_\ell \hat{H} = [\hat{\eta}, \hat{H}] \quad , \quad \text{with} \quad \hat{H} \equiv \begin{pmatrix} H & A^\dagger \\ A & O \end{pmatrix} \quad , \quad \hat{\eta} \equiv \begin{pmatrix} \eta & -\bar{\eta}^\dagger \\ \bar{\eta} & \eta \end{pmatrix} \quad . \tag{6.1}$$

The auxiliary operator A and the additional generator $\bar{\eta}$ can now be chosen such that certain sum rules for the observable O hold.

There are some physical models to which the methods developed in this work can be applied. To treat an electron-phonon system in an external potential, one can start from the electron-phonon system discussed in Ref. [Len96] and add an potential that confines the electrons, say. Following the truncation scheme outlined in Chapter 3, the distinguished bosonic modes are then given by $\bar{a}_q \equiv a_q + \sum_k M_{k,q}/\omega_q \langle c_k^\dagger c_{k+q}\rangle$, using the notations of Ref. [Len96]. This different truncation scheme may lead to a modified effective electron-electron coupling.

Another interesting model would be the Tomonaga-Luttinger Model in an external potential. The Flow Equations are similar to the ones for the impurity, but interference effects may lead to a different physical behaviour of the system with a finite impurity.

A. Normal Ordering

In this Appendix we want to summarize basic relations concerning normal ordering. This summary is based on unpublished notes by Wegner of the year 2000 in which he presents a general formalism for normal ordering of classical and quantum fields with respect to a bilinear Hamiltonian. Wegner refers to the Refs. [Wic50], [Zin80] and [Weg76]. We will restrain ourselves to the normal ordering of quantum fields.

A.1. Bosons

Let a_k be any linear combination of Bose creation and annihilation operators. The matrix G shall describe the correlations of the operators a for a Hamiltonian H bilinear in the creation and annihilation operators: $\langle a_k a_l \rangle = G_{kl}$. The commutator is given by $[a_k, a_l] = G_{kl} - G_{lk}$. Normal ordering of an operator A with respect to the Hamiltonian H is now defined by:

$$:1: = 1 \tag{A.1}$$

$$:\alpha A(a) + \beta B(a): = \alpha : A(a) : + \beta : B(a): \tag{A.2}$$

$$a_k : A(a) : =: a_k A(a) : + \sum_l G_{kl} : \frac{\partial A(a)}{\partial a_k} : \tag{A.3}$$

The product of m operators a_{k_i} with $i = 1..m$ is now obtained by iterating the third equation. One obtains

$$a_{k_1} a_{k_2} ... a_{k_m} =: (a_{k_1} + \sum_{l_1} G_{k_1,l_1} \frac{\partial}{\partial a_{l_1}})(a_{k_2} + \sum_{l_2} G_{k_2,l_2} \frac{\partial}{\partial a_{l_2}}) ... a_{k_m} : \quad , \tag{A.4}$$

which can also be written as

$$a_{k_1} a_{k_2} ... a_{k_m} =: \exp(\sum_{kl} G_{kl} \frac{\partial^2}{\partial a_k^{left} \partial a_l^{right}}) a_{k_1} a_{k_2} ... a_{k_m} : \quad . \tag{A.5}$$

This is Wick's first theorem. The superscripts ^{left} and ^{right} indicate that we always pick a pair of factors a and perform the derivative $\partial/\partial a_k$ on the left factor and the derivative $\partial/\partial a_l$ on the right factor, so that the factor G_{kl} depends on the sequence of the operators.

Similarly one obtains

$$: a_{k_1} a_{k_2} ... a_{k_m} := \exp(-\sum_{kl} G_{kl} \frac{\partial^2}{\partial a_k^{left} \partial a_l^{right}}) a_{k_1} a_{k_2} ... a_{k_m} \quad . \tag{A.6}$$

The formula for the product of two normal ordered operators is given by

$$: A(a) :: B(a) :=: \exp(\sum_{kl} G_{kl} \frac{\partial^2}{\partial a_k \partial b_l}) A(a) B(b) : |_{b=a} \quad . \tag{A.7}$$

This is Wicks's second theorem.

One can now show that under normal ordering the commutative law holds: $: ABCD :=: ACBD :$. This is rule C of Wick.

A.2. Fermions

For fermions one can basically use the same reasoning. But since fermions anti-commute, one now has to replace the commutator in the bosonic case by the anti-commutator: $\{a_k, a_l\} = G_{kl} + G_{lk}$. It also has to be observed that $(\partial/\partial a_l) a_k = \delta_{k,l} - a_k \partial/\partial a_l$ and that in the second derivatives in the exponentials the derivative with respect to a^{left} has to be performed before a^{right}. Thus Wick's theorem of Eq. (A.7) has to be written as

$$: A(a) :: B(a) :=: \exp(\sum_{kl} G_{kl} \frac{\partial^2}{\partial b_l \partial a_k}) A(a) B(b) : |_{b=a} \quad . \tag{A.8}$$

The commutative law under normal ordering then reads $: ABCD := \pm : ACBD :$, where the minus sign applies if B and C are both odd elements of the algebra and the plus sign if B or C is an even element.

B. Two-Level System

The two-level system shall be described by the one-particle Hamiltonian

$$H_S = -\frac{\Delta}{2}\sigma_x + \epsilon c_1^\dagger c_1 \quad . \tag{B.1}$$

The matrix representation is given by the following 2×2-matrix:

$$H_S = \begin{pmatrix} 0 & -\Delta/2 \\ -\Delta/2 & \epsilon \end{pmatrix} \tag{B.2}$$

The eigenvalues are given by $\lambda_\pm = \epsilon/2 \pm R/2$ with the Rabi-frequency $R \equiv \sqrt{\epsilon^2 + \Delta^2}$. The normalized eigenvectors are thus given by

$$\vec{v}_\pm \equiv \sqrt{\frac{\Delta}{2R}} \begin{pmatrix} \sqrt{\frac{\Delta}{R \pm \epsilon}} \\ \mp\sqrt{\frac{R \pm \epsilon}{\Delta}} \end{pmatrix} \quad . \tag{B.3}$$

This yields the following expectation values for the Pauli spin matrices:

$$\langle \sigma_x \rangle = \frac{\Delta}{R} \quad , \quad \langle \sigma_y \rangle = 0 \quad , \quad \langle \sigma_z \rangle = \frac{\epsilon}{R} \quad . \tag{B.4}$$

The operator $c_1^\dagger c_1$ transforms under the unitary transformation

$$H_S \to \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \tag{B.5}$$

as $c_1^\dagger c_1 \to \frac{1}{2} - \frac{\Delta}{2R}\sigma_x + \frac{\epsilon}{2R}\sigma_z$.

In order to complete the discussion we also consider the the symmetric version of the two-level system:

$$H_S = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z \tag{B.6}$$

Since $\sigma_z = 1 - 2c_1^\dagger c_1$ the eigenvalues are shifted to yield $\lambda_\pm = \pm R/2$ and the new eigenvectors and expectation values are obtained by replacing $\epsilon \to -\epsilon$ in the above equations. Thus, the operator σ_z transforms as $\sigma_z \to \frac{\Delta}{R}\sigma_x + \frac{\epsilon}{R}\sigma_z$.

C. Rabi Model in Perturbation Theory

In this Appendix we will treat the Rabi Hamiltonian in perturbation theory. We want to start from the exactly solvable Jaynes-Cummings Hamiltonian which is obtained from the Rabi Hamiltonian by applying the rotating wave approximation [Jay63]. This approximation neglects coupling or transition terms which are energetically unlikely.

It is useful to write the Hamiltonian in a basis where σ_x is diagonal. The Rabi Hamiltonian shall thus be given by

$$H = \sum_{i=0,1} \epsilon_i c_i^\dagger c_i + \omega_0 b^\dagger b + \lambda b c_1^\dagger c_0 + \lambda b^\dagger c_0^\dagger c_1 + \lambda' b^\dagger c_1^\dagger c_0 + \lambda' b c_0^\dagger c_1 \quad . \tag{C.1}$$

The operators $c_i^{(\dagger)}$ and $b^{(\dagger)}$ obey the canonical anti-commutation and commutation relations respectively. We identify the Rabi Hamiltonian given in Eq. (3.1) by setting $\epsilon_1 - \epsilon_0 = \Delta_0$ and $\lambda = \lambda' = 2\lambda_0$.

The Jaynes-Cummings Hamiltonian is obtained by setting $\lambda' = 0$ in Eq. (C.1). We want to treat the so called off-shell processes, characterized by λ', within a systematic perturbation approach. One way to do so is to consider the Hamiltonian in the basis $\{|0;2n\rangle|1;2n+1\rangle\}$ and $\{|0;2n+1\rangle, |1;2n\rangle\}$ where the first quantum number resembles the fermionic state and the second quantum number the bosonic state. Since the Hamiltonian is symmetric with respect to parity the two sets decouple and in the following we will only consider the first set.

Let us define the n-dependent matrices

$$\begin{aligned} D^{\text{on}}(n) &\equiv \begin{pmatrix} \epsilon_1 + 2n\omega_0 & \sqrt{2n+1}\lambda \\ \sqrt{2n+1}\lambda & D^{\text{off}}(n+1) \end{pmatrix} \quad , \\ D^{\text{off}}(n+1) &\equiv \begin{pmatrix} \epsilon_0 + (2n+1)\omega_0 & \sqrt{2n+2}\lambda' \\ \sqrt{2n+2}\lambda' & D^{\text{on}}(n+1) \end{pmatrix} \quad . \end{aligned} \tag{C.2}$$

The determinants can formally be evaluated to yield

$$\begin{aligned} \det D^{\text{on}}(n) &= (\epsilon_1 + 2n\omega_0)\det D^{\text{off}}(n+1) - (2n+1)\lambda^2 \det D^{\text{on}}(n+1) \\ \det D^{\text{off}}(n+1) &= (\epsilon_0 + (2n+1)\omega_0)\det D^{\text{on}}(n+1) - (2n+2)\lambda'^2 \det D^{\text{off}}(n+2) \quad . \end{aligned} \tag{C.3}$$

The matrix $D^{\text{on}}(0)$ resembles the representation of the Rabi Hamiltonian in the above basis. To determine the eigenvalue μ of the matrix up to $O(\lambda'^2)$ we iterate Eq.

(C.3) starting with $D^{\mathrm{on}}(0)$:

$$\begin{aligned}\det(D^{\mathrm{on}}(0)-\mu) \to & \left[(\epsilon_1-\mu)(\epsilon_0+\omega_0-\mu)-\lambda^2\right] \\ & \times\left[(\epsilon_1+2\omega_0-\mu)(\epsilon_0+3\omega_0-\mu)-3\lambda^2\right]\det(D^{\mathrm{on}}(2)-\mu) \\ & -(\epsilon_1-\mu)2\lambda'^2(\epsilon_0+3\omega_0-\mu)\det(D^{\mathrm{on}}(2)-\mu)=0\end{aligned} \tag{C.4}$$

For the eigenvalues we make the ansatz $\mu=\mu^{(0)}+\lambda'^2\mu^{(1)}$. There is no linear term in λ' since the spectrum of H may not depend on the phase of the coupling constant.

We now order the eigenvalues as follows: The lowest eigenvalue of order $O(\lambda'^0)$ $\mu_0^{(0)}$ is determined by setting the first factor on the right hand side of Eq. (C.4) zero. We obtain the well-known James-Cummings result $\mu_0^{(0)}=\epsilon_0+\omega_0-(\bar{\Delta}\mp R_0)/2$ with the detuning $\bar{\Delta}\equiv(\epsilon_1-\epsilon_0)-\omega_0$ and the zeroth Rabi frequency $R_0^2=\bar{\Delta}^2+4\lambda^2$. The first correction to $\mu_0^{(0)}$ then yields

$$\mu_0^{(1)}=\frac{1}{\mp R_0}\frac{\bar{\Delta}\omega_0\pm R_0\omega_0-\lambda^2}{2\omega_0^2\mp R_0\omega_0-\lambda^2} \quad . \tag{C.5}$$

The result agrees with the perturbative result in the limit $\lambda=\lambda'\ll\bar{\Delta}$.

Generally, setting the nth factor of the first line on the right hand side of Eq. (C.4) zero the nth eigenvalue yields $\mu_n^{(0)}=\epsilon_0+(2n+1)\omega_0-(\bar{\Delta}\mp R_n)/2$ with $R_n^2=\bar{\Delta}^2+4(2n+1)\lambda^2$. The first correction to $\mu_n^{(0)}$ is given by

$$\begin{aligned}\mu_n^{(1)}=\frac{1}{\mp R_n}\Bigg[&(n+1)\frac{\bar{\Delta}\omega_0\pm R_n\omega_0-\lambda^2}{2\omega_0^2\mp R_n\omega_0-(n+1)\lambda^2} \\ &+n\frac{\bar{\Delta}\omega_0\mp R_n\omega_0-\lambda^2}{2\omega_0^2\pm R_n\omega_0-(n-1)\lambda^2}\Bigg] \quad .\end{aligned} \tag{C.6}$$

The perturbative approach breaks down when there are degenerated states. This is indicated by the poles in the energy corrections $\mu_n^{(1)}$. Considering the pole of $\mu_0^{(1)}$ one obtains for the tunnel-matrix element $\Delta_0=\omega_0+\sqrt{(2\omega_0-\lambda^2)^2-4\omega_0^2\lambda^2}/\omega_0$. Inserting the parameters of Fig. 3.6 we obtain $\Delta_0\approx 2.87$. This value approximately agrees with the value of Δ_0 where the second spike of h_z in Figure 3.6 is seen.

D. Spin-Boson Model with Spontaneously Broken Symmetry

In this Appendix we will set up Flow Equations for the Spin-Boson Model employing a representation which explicitly breaks the reflection symmetry. We embark from the Spin-Boson Hamiltonian which is usually given by

$$H = -\frac{\Delta}{2}\sigma_x + \sum_\alpha \omega_\alpha (b_\alpha^\dagger + \sigma_z \frac{\lambda_\alpha}{2\omega_\alpha})(b_\alpha + \sigma_z \frac{\lambda_\alpha}{2\omega_\alpha}) + E_0 \quad . \tag{D.1}$$

The operators $b_\alpha^{(\dagger)}$ resemble the bath degrees of freedom and σ_i with $i = x, y, z$ denote the Pauli spin matrices. They obey the canonical commutation relations and the spin-1/2 algebra respectively. In the following we will also use a decomposed representation of the Pauli spin matrices: $\sigma_x \equiv c_1^\dagger c_0 + c_0^\dagger c_1$, $-i\sigma_y \equiv c_1^\dagger c_0 - c_0^\dagger c_1$ and $\sigma_z \equiv c_0^\dagger c_0 - c_1^\dagger c_1$. The $c_i^{(\dagger)}$ obey the canonical anti-commutation relations. Further we have $1 = c_0^\dagger c_0 + c_1^\dagger c_1$.

The Spin-Boson Hamiltonian exhibits the discrete symmetry $c_0 \to c_1$, $c_1 \to c_0$ and $b_\alpha^{(\dagger)} \to -b_\alpha^{(\dagger)}$ which can be thought of as reflection symmetry. The Hamiltonian thus commutes with the symmetry operator and we can therefore label the eigenstates as $|\pm, r\rangle$, where $\pm$ defines the parity and r stands for further quantum numbers. If the generator does not break the reflection symmetry, this holds for all ℓ so that the true spectrum for small Ohmic coupling, consisting of a non-degenerate ground-state plus a "pure" continuum, will not be recovered for any finite ℓ. It is thus crucial to transform the Hamiltonian in such a way that this discrete symmetry is "spontaneously" broken. To do so it is convenient to translate the bosonic modes $b_\alpha \to b_\alpha - \lambda_\alpha/(2\omega_\alpha)$. With

$$U = \exp(-\sum_\alpha \frac{\lambda_\alpha}{2\omega_\alpha}(b_\alpha - b_\alpha^\dagger)) \tag{D.2}$$

we obtain the unitary equivalent Hamiltonian $H \leftarrow UHU^\dagger$

$$\begin{aligned} H &= -\frac{\Delta}{2}\sigma_x + \sum_\alpha \omega_\alpha (b_\alpha^\dagger - c_1^\dagger c_1 \frac{\lambda_\alpha}{\omega_\alpha})(b_\alpha - c_1^\dagger c_1 \frac{\lambda_\alpha}{\omega_\alpha}) + E_0 \\ &= -\frac{\Delta}{2}\sigma_x + \sum_\alpha \omega_\alpha b_\alpha^\dagger b_\alpha - c_1^\dagger c_1 \sum_\alpha \lambda_\alpha (b_\alpha + b_\alpha^\dagger) + c_1^\dagger c_1 \Lambda + E_0 \quad , \end{aligned} \tag{D.3}$$

where we defined $\Lambda \equiv \sum_\alpha \lambda_\alpha^2/\omega_\alpha$.

The generator η of the infinitesimal unitary transformations is chosen to be

$$\begin{aligned}\eta = \eta^y i\sigma_y + \sum_\alpha \eta_\alpha^e(b_\alpha - b_\alpha^\dagger) + i\sigma_y \sum_\alpha \eta_\alpha^y(b_\alpha + b_\alpha^\dagger) + \sigma_z \sum_\alpha \eta_\alpha^z(b_\alpha - b_\alpha^\dagger) \\ + \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}(b_\alpha + b_\alpha^\dagger)(b_{\alpha'} - b_{\alpha'}^\dagger) \equiv \eta^{y,0} + \eta^{e,1} + \eta^{y,1} + \eta^{z,1} + \eta_B \quad .\end{aligned} \tag{D.4}$$

In fact we just transformed the generator employed to diagonalize the initial Spin-Boson Hamiltonian in subsection 4.2.1 by the same unitary transformation (D.2) and generalized the coefficients.

The commutator $[\eta, H]$ yields the following contributions:

$$[\eta^{y,0}, H] = -\Delta\eta^y\sigma_z - \eta^y\sigma_x \sum_\alpha \lambda_\alpha(b_\alpha + b_\alpha^\dagger) + \eta^y\sigma_x\Lambda \tag{D.5}$$

$$[\eta^{e,1}, H] = \sum_\alpha \eta_\alpha^e\omega_\alpha(b_\alpha + b_\alpha^\dagger) - 2c_1^\dagger c_1 \sum_\alpha \eta_\alpha^e\lambda_\alpha \tag{D.6}$$

$$\begin{aligned}[\eta^{y,1}, H] = &-\Delta\sigma_z \sum_\alpha \eta_\alpha^y(b_\alpha + b_\alpha^\dagger) + i\sigma_y \sum_\alpha \eta_\alpha^y\omega_\alpha(b_\alpha - b_\alpha^\dagger) \\ &- \sigma_x \sum_{\alpha,\alpha'} \eta_\alpha^y\lambda_{\alpha'}(b_\alpha + b_\alpha^\dagger)(b_{\alpha'} + b_{\alpha'}^\dagger) + \sigma_x \sum_\alpha \eta_\alpha^y(b_\alpha + b_\alpha^\dagger)\Lambda\end{aligned}$$

$$[\eta^{z,1}, H] = -i\sigma_y\Delta \sum_\alpha \eta_\alpha^z(b_\alpha - b_\alpha^\dagger) + \sigma_z \sum_\alpha \eta_\alpha^z\omega_\alpha(b_\alpha + b_\alpha^\dagger) + 2c_1^\dagger c_1 \sum_\alpha \eta_\alpha^z\lambda_\alpha \tag{D.7}$$

$$\begin{aligned}[\eta_B, H] = &\sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}\omega_\alpha(b_\alpha - b_\alpha^\dagger)(b_{\alpha'} - b_{\alpha'}^\dagger) + \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}\omega_{\alpha'}(b_\alpha + b_\alpha^\dagger)(b_{\alpha'} + b_{\alpha'}^\dagger) \\ &- 2c_1^\dagger c_1 \sum_{\alpha,\alpha'} \eta_{\alpha,\alpha'}\lambda_{\alpha'}(b_\alpha + b_\alpha^\dagger)\end{aligned} \tag{D.8}$$

We introduced $\Lambda(\ell)$ with the initial condition $\Lambda(\ell = 0) \equiv \sum_\alpha \frac{\lambda_\alpha^2(\ell=0)}{\omega_\alpha}$ to emphasize that it might differ from $\widetilde{\Lambda}(\ell) \equiv \sum_\alpha \frac{\lambda_\alpha^2(\ell)}{\omega_\alpha}$ during the flow. We will see that this is only the case if we introduce a bias $\epsilon c_1^\dagger c_1$ to the Hamiltonian (D.3).

It is now crucial to truncate the Flow Equations with respect to the distinguished modes. Since the bosonic operators are shifted by $-c_1^\dagger c_1\lambda_\alpha/\omega_\alpha$ we will define normal ordering with respect to the ground-state of

$$H_B = \sum_\alpha \omega_\alpha(b_\alpha^\dagger - \langle c_1^\dagger c_1\rangle\frac{\lambda_\alpha}{\omega_\alpha})(b_\alpha - \langle c_1^\dagger c_1\rangle\frac{\lambda_\alpha}{\omega_\alpha}) \quad . \tag{D.9}$$

Normal ordering of the system operators is done with respect to $H_S = -\frac{\Delta_r}{2}\sigma_x + (\Lambda - \widetilde{\Lambda})c_1^\dagger c_1$, where the renormalized tunnel-matrix element Δ_r can include bath properties. We thus introduce a ℓ-dependent normal ordering which is twofold; first it depends on the flow of the coupling parameters λ_α, but it also depends on the flow of the system parameters through the expectation values $\langle c_1^\dagger c_1\rangle$ and $\langle\sigma_x\rangle$.

So neglecting the normal ordered operator $:\sigma_x: \sum_{\alpha,\alpha'}\eta^y_\alpha\lambda_{\alpha'}\ :(:(b_\alpha+b^\dagger_\alpha):$ $:(b_{\alpha'}+b^\dagger_{\alpha'}):):$, the constants have to satisfy the following relations in order that the Hamiltonian (D.3) remains form-invariant:

$$\eta^z_\alpha\Delta-\eta^y_\alpha\omega_\alpha=0 \tag{D.10}$$

$$\eta^e_\alpha\omega_\alpha+\eta^z_\alpha\omega_\alpha-\eta^y_\alpha\Delta+\textstyle\sum_{\alpha'}(\eta_{\alpha,\alpha'}\omega_{\alpha'}+\eta_{\alpha',\alpha}\omega_\alpha)\langle(b_{\alpha'}+b^\dagger_{\alpha'})\rangle=0 \tag{D.11}$$

$$\eta^y\lambda_\alpha-\eta^y_\alpha\Lambda+\textstyle\sum_{\alpha'}(\eta^y_\alpha\lambda_{\alpha'}+\eta^y_{\alpha'}\lambda_\alpha)\langle(b_{\alpha'}+b^\dagger_{\alpha'})\rangle=0 \tag{D.12}$$

$$\eta_{\alpha,\alpha'}\omega_\alpha+\eta_{\alpha',\alpha}\omega_{\alpha'}=0 \tag{D.13}$$

$$\eta_{\alpha,\alpha'}\omega_{\alpha'}+\eta_{\alpha',\alpha}\omega_\alpha-(\eta^y_\alpha\lambda_{\alpha'}+\eta^y_{\alpha'}\lambda_\alpha)\langle\sigma_x\rangle=0 \tag{D.14}$$

Eqs. (D.10) guarantees that operators of the form $i\sigma_y p_\alpha$ are not created during the flow. Eqs. (D.11) account for the vanishing of x_α, Eqs. (D.12) for $\sigma_x x_\alpha$, Eqs. (D.13) for $:p_\alpha p_\alpha:$ and Eqs. (D.14) for $:(:x_\alpha:)(:x_\alpha:):$, where we introduced $x_\alpha\equiv(b_\alpha+b^\dagger_\alpha)$ and $p_\alpha\equiv(b_\alpha-b^\dagger_\alpha)$. Notice that from Eqs. (D.13) there follows $\eta_{\alpha,\alpha'}=0$. This will allow us to interpret later integrals as principal value integrals.

With these equations the constants are defined up to a constant which will set the scale of the ℓ-flow, and we obtain the following Flow Equations:

$$\partial_\ell\Delta=2\sum_\alpha\eta^y_\alpha\lambda_\alpha(2n_\alpha+1)-2C\Lambda-2\sum_{\alpha,\alpha'}\eta^y_\alpha\lambda_{\alpha'}\langle(b_\alpha+b^\dagger_\alpha)\rangle\langle(b_{\alpha'}+b^\dagger_{\alpha'})\rangle \tag{D.15}$$

$$\partial_\ell\Lambda=2\sum_\alpha\eta^z_\alpha\lambda_\alpha+2\Delta C-2\sum_\alpha\eta^e_\alpha\lambda_\alpha \tag{D.16}$$

$$\partial_\ell\lambda_\alpha=2\eta^z_\alpha\omega_\alpha-2\Delta\eta^y_\alpha+2\sum_{\alpha'}\eta_{\alpha,\alpha'}\lambda_{\alpha'} \tag{D.17}$$

$$\partial_\ell E_0=-\Delta C+\sum_{\alpha,\alpha'}\eta_{\alpha,\alpha'}\langle(b_\alpha+b^\dagger_\alpha)\rangle\langle(b_{\alpha'}+b^\dagger_{\alpha'})\rangle \tag{D.18}$$

If one chooses the free factor such that $\eta^y_\alpha=-\Delta\lambda_\alpha/2$ one finds with $\langle(b_\alpha+b^\dagger_\alpha)\rangle=2\langle c_1^\dagger c_1\rangle\lambda_\alpha/\omega_\alpha$ that $\eta^z_\alpha=-\omega_\alpha\lambda_\alpha/2$, $\eta^e_\alpha=-\Delta^2\lambda_\alpha/\omega_\alpha/2+\lambda_\alpha\omega_\alpha/2+(2\langle c_1^\dagger c_1\rangle)\langle\sigma_x\rangle\Delta\widetilde{\Lambda}\lambda_\alpha/\omega_\alpha$, $\eta^y=-\Delta\Lambda/2+(2\langle c_1^\dagger c_1\rangle)\Delta\widetilde{\Lambda}$, $\eta_{\alpha,\alpha'}=\Delta\langle\sigma_x\rangle\lambda_\alpha\lambda_{\alpha'}\omega_{\alpha'}/(\omega_\alpha^2-\omega_{\alpha'}^2)$. Introducing the spectral function

$$J(\omega)=\sum_\alpha\lambda_\alpha^2\delta(\omega-\omega_\alpha)\quad, \tag{D.19}$$

one obtains the following coupled integro-differential equations:

$$\partial_\ell \Delta = -\Delta \int d\omega J(\omega,\ell)(2n(\omega)+1) + \Delta(\Lambda - 2\langle c_1^\dagger c_1\rangle \widetilde{\Lambda})^2 \tag{D.20}$$

$$\begin{aligned}\partial_\ell \Lambda = &-2\int d\omega J(\omega,\ell)\omega - \Delta^2\Lambda + \Delta^2\widetilde{\Lambda} \\ &+ 2(2\langle c_1^\dagger c_1\rangle)(\Delta^2\widetilde{\Lambda} - \langle\sigma_x\rangle\Delta\widetilde{\Lambda}^2)\end{aligned} \tag{D.21}$$

$$\partial_\ell J(\omega,\ell) = 2J(\omega,\ell)(\Delta^2-\omega^2) + 4\Delta\langle\sigma_x\rangle J(\omega,\ell)\int d\omega' \frac{J(\omega',\ell)\omega'}{\omega^2-\omega'^2} \tag{D.22}$$

Dividing Eq. (D.22) by ω, integrating over ω and using the identity

$$\int d\omega \int d\omega' \frac{J(\omega)J(\omega')}{\omega\omega'}\frac{\omega'^2}{\omega^2-\omega'^2} = -\frac{1}{2}\int d\omega\int d\omega' \frac{J(\omega)J(\omega')}{\omega\omega'} \tag{D.23}$$

we can write Eq. (D.21) as

$$\partial_\ell \epsilon = -\Delta^2\epsilon + 2(2\langle c_1^\dagger c_1\rangle - 1)(\Delta^2\widetilde{\Lambda} - \langle\sigma_x\rangle\Delta\widetilde{\Lambda}^2) \quad , \tag{D.24}$$

where we introduced the bias $\epsilon = \Lambda - \widetilde{\Lambda}$. These are the same Flow Equations as in Eqs. (4.69) - (4.71).

We now turn to the expectation values characterizing the system. They can be given by

$$2\langle c_1^\dagger c_1\rangle = 1 - \frac{\epsilon}{\sqrt{\Delta_r^2+\epsilon^2}} \quad , \quad \langle\sigma_x\rangle = \frac{\Delta_r}{\sqrt{\Delta_r^2+\epsilon^2}} \quad . \tag{D.25}$$

For super-Ohmic baths the renormalized tunnel matrix element can be given by $\Delta_r \equiv \Delta\exp(-\sum_\alpha \frac{\lambda_\alpha^2}{2\omega_\alpha^2})$. Otherwise we introduce no renormalization, i.e. $\Delta_r \equiv \Delta$.

Keeping in mind that the cutoff frequency of the spectral function ω_c sets the largest energy scale, i.e. $\omega_c \gg \Delta$, we observe that for $1/\Delta^2 \gg \ell$ the fixed line $\epsilon = 0$ is stable for super-Ohmic baths and instable otherwise. For $1/\Delta^2 \ll \ell$ it resembles a stable fixed line for all bath types.

E. Dissipative Particle in a Periodic Tight-Binding Potential

To describe a quantum mechanical Brownian particle in a periodic tight-binding potential we shall start with the following Hamiltonian:

$$\begin{aligned} H = &-\frac{\Delta}{2}\sum_n (c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1}) + \sum_\alpha \omega_\alpha b^\dagger_\alpha b_\alpha + q_0^2 \sum_n n^2 c^\dagger_n c_n \Lambda \\ &- q_0 \sum_n n c^\dagger_n c_n \sum_\alpha \lambda_\alpha (b_\alpha + b^\dagger_\alpha) - H' \end{aligned} \tag{E.1}$$

The additional contribution to the Hamiltonian H' shall be zero at $\ell = 0$ and is defined as

$$H' \equiv q_0 \sum_n (c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1}) \sum_\alpha \lambda'_\alpha (b_\alpha + b^\dagger_\alpha) \quad . \tag{E.2}$$

The operators $b_\alpha^{(\dagger)}$ resemble the bath degrees of freedom and $c_n^{(\dagger)}$ are the creation and annihilation operators of the Wannier state at lattice site n. They obey the canonical commutation and anti-commutation relations respectively. Further we defined $\Lambda \equiv \sum_\alpha \lambda_\alpha^2/\omega_\alpha$. In the following summation over the bath modes α and the Fourier modes n is implied.

The generator η of the infinitesimal unitary transformations is chosen to be

$$\begin{aligned} \eta = &\, n c^\dagger_n c_n \eta^q_\alpha (b_\alpha - b^\dagger_\alpha) + (c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1}) \eta^p_\alpha (b_\alpha + b^\dagger_\alpha) \\ &+ \eta_{\alpha,\alpha'} (b_\alpha + b^\dagger_\alpha)(b_{\alpha'} - b^\dagger_{\alpha'}) \equiv \eta^q + \eta^p + \eta_B \quad . \end{aligned} \tag{E.3}$$

The first two terms η^q and η^p stem from the canonical choice of the generator $\eta = [H_0, V]$ with generalized parameters. The last term η_B is needed for eliminating the coupling term between the bath modes.

The commutator $[\eta, H]$ yields the following contributions:

$$
\begin{aligned}
[\eta^q, H] &= -\frac{\Delta}{2}(c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1})\eta^q_\alpha(b_\alpha - b^\dagger_\alpha) \qquad \text{(E.4)}\\
&\quad + nc^\dagger_n c_n \eta^q_\alpha \omega_\alpha(b_\alpha + b^\dagger_\alpha) - 2q_0(nc^\dagger_n c_n)^2\eta^q_\alpha\lambda_\alpha\\
[\eta^p, H] &= (c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1})\eta^p_\alpha\omega_\alpha(b_\alpha - b^\dagger_\alpha) \qquad \text{(E.5)}\\
&\quad + q_0(c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1})\eta^p_\alpha\lambda_{\alpha'}(b_\alpha + b^\dagger_\alpha)(b_{\alpha'} + b^\dagger_{\alpha'})\\
&\quad - q_0^2\big(nc^\dagger_n c_n(c^\dagger_{n'+1}c_{n'} + c^\dagger_{n'}c_{n'+1}) + h.c.\big)\eta^p_\alpha(b_\alpha + b^\dagger_\alpha)\Lambda\\
[\eta_B, H] &= \eta_{\alpha,\alpha'}\omega_\alpha(b_\alpha - b^\dagger_\alpha)(b_{\alpha'} - b_{\alpha'}) + \eta_{\alpha,\alpha'}\omega_{\alpha'}(b_\alpha + b^\dagger_\alpha)(b_{\alpha'} + b^\dagger_{\alpha'})\\
&\quad - 2q_0 nc^\dagger_n c_n \eta_{\alpha,\alpha'}\lambda_{\alpha'}(b_\alpha + b^\dagger_\alpha) \qquad \text{(E.6)}\\
[\eta^q, H'] &= (c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1})\eta^q_\alpha\lambda_{\alpha'}(b_\alpha - b^\dagger_\alpha)(b_{\alpha'} + b^\dagger_{\alpha'}) \qquad \text{(E.7)}\\
&\quad + (c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1})\eta^q_\alpha\lambda_\alpha(b_\alpha b_\alpha - b^\dagger_\alpha b^\dagger_\alpha)\\
&\quad + \big(nc^\dagger_n c_n(c^\dagger_{n'+1}c_{n'} + c^\dagger_{n'}c_{n'+1}) + h.c.\big)\Lambda\\
[\eta_B, H'] &= -2(c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1})\eta_{\alpha,\alpha'}\lambda_{\alpha'}(b_\alpha + b^\dagger_\alpha) \qquad \text{(E.8)}
\end{aligned}
$$

In order to close the Flow Equations we will have to make one approximation

$$n^2 c^\dagger_n c_n \to 2\sqrt{\langle q^2\rangle}\, nc^\dagger_n c_n \quad , \qquad \text{(E.9)}$$

where we defined $\langle q^2\rangle \equiv \langle n^2 c^\dagger_n c_n\rangle$, with $\langle ...\rangle$ denoting the ground-state expectation value with respect to the effective one-particle Hamiltonian. If we restrict ourselves to the one-particle Hilbert space so that $(nc^\dagger_n c_n)^2 = n^2 c^\dagger_n c_n$ holds, we can then write

$$
\begin{aligned}
&\big(nc^\dagger_n c_n(c^\dagger_{n'+1}c_{n'} + c^\dagger_{n'}c_{n'+1}) + h.c.\big) = [c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1}, (n'c^\dagger_{n'}c_{n'})^2]\\
&\to 2\sqrt{\langle q^2\rangle}[c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1}, n'c^\dagger_{n'}c_{n'}] = 2\sqrt{\langle q^2\rangle}(c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1}) \quad .
\end{aligned}
\qquad \text{(E.10)}
$$

For the Hamiltonian to remain form-invariant the constants have to satisfy the following relations:

$$\eta^q_\alpha\Delta + \eta^p_\alpha\omega_\alpha = 0 \qquad \text{(E.11)}$$

$$\eta_{\alpha,\alpha'}\omega_\alpha + \eta_{\alpha',\alpha}\omega_{\alpha'} = 0 \qquad \text{(E.12)}$$

$$\eta_{\alpha,\alpha'}\omega_{\alpha'} + \eta_{\alpha',\alpha}\omega_\alpha - (\eta^p_\alpha\lambda_{\alpha'} + \eta^p_{\alpha'}\lambda_\alpha)\langle(c^\dagger_{n+1}c_n + c^\dagger_n c_{n+1})\rangle = 0 \qquad \text{(E.13)}$$

The Flow Equations are thus given by

$$\partial_\ell\Delta = -q_0 2\sqrt{\langle q^2\rangle}\eta^q_\alpha\lambda'_\alpha \quad , \quad \partial_\ell\Lambda = -\frac{2}{q_0}\eta^q_\alpha\lambda_\alpha \qquad \text{(E.14)}$$

$$\partial_\ell\lambda_\alpha = -\frac{1}{q_0}\eta^q_\alpha\omega_\alpha + 2\eta_{\alpha,\alpha'}\lambda_{\alpha'} \quad , \quad \partial_\ell\lambda'_\alpha = -q_0 2\sqrt{\langle q^2\rangle}\eta^p_\alpha\frac{\lambda^2_\alpha}{\omega_\alpha} + 2\eta_{\alpha,\alpha'}\lambda'_{\alpha'} \quad . \qquad \text{(E.15)}$$

We did not investigate these Flow Equations further.

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